4-2012

Renewable Para-Xylene

Eric Castillo  
*University of Pennsylvania*

Tyler Ernst  
*University of Pennsylvania*

Corey Lerch  
*University of Pennsylvania*

J. Parker Winchester  
*University of Pennsylvania*

Follow this and additional works at: [http://repository.upenn.edu/cbe_sdr](http://repository.upenn.edu/cbe_sdr)

Castillo, Eric; Ernst, Tyler; Lerch, Corey; and Winchester, J. Parker, "Renewable Para-Xylene" (2012). *Senior Design Reports (CBE)*. 36.  
[http://repository.upenn.edu/cbe_sdr/36](http://repository.upenn.edu/cbe_sdr/36)

This paper is posted at Scholarly Commons. [http://repository.upenn.edu/cbe_sdr/36](http://repository.upenn.edu/cbe_sdr/36)

For more information, please contact libraryrepository@pobox.upenn.edu.
Renewable Para-Xylene

Abstract
This report details a process designed to renewably produce 400 million pounds of para-xylene per year from corn dry grind, sugar cane molasses (SCM), or woody biomass while minimizing water use. The para-xylene should be suitable for the production of polymers and plastics, and should be economical and green. All three feedstocks are equally suitable for the process and available for use.

The process is designed for SCM and consumes a total feed of 9.35 billion pounds of molasses per year. Corn dry grind is simply too expensive, and biomass, while cheaper per pound, imposes too many additional pre-processing costs. The molasses first undergoes hydrolysis then hydrogenation, followed by condensation and separation involving distillation and crystallization. Transalkylation and aqueous phase reforming are also employed to boost yield and create a self-contained process.

Several key assumptions are inherent in this process’s design. First, all reactor yields come directly from specific examples in the literature. Second, results found in the patents for glycerol were assumed valid for sorbitol as well, since not all patents used the same materials for their examples. Third, the economic analysis assumes that raw materials for catalyst manufacture can be purchased in bulk for a quarter of the price for small quantities. This assumption was suggested by Dr. Fabiano.

Based on these assumptions, the process designed herein meets the desired non-financial criteria, but results in an investor’s rate of return of negative 2.90% and a net present value of negative $196 million. However, further research into the catalyst or reactor yields could easily allow the process to break even or offer an attractive return.

This working paper is available at ScholarlyCommons: http://repository.upenn.edu/cbe_sdr/36
Renewable Para-Xylene

Senior Design Project

Eric Castillo, Tyler Ernst, Corey Lerch, J. Parker Winchester

4/10/2012

Department of Chemical and Biomolecular Engineering
University of Pennsylvania

Faculty Advisor: Dr. Miriam Wattenbarger, University of Pennsylvania
Project Author: Mr. Stephen M. Tieri, DuPont Engineering Research & Technology
Dear Dr. Wattenbarger, Dr. Fabiano, and Mr. Stephen Tieri,

Following our original Senior Design Project Statement, we have designed a process for the renewable production of para-xylene, enclosed herein. As requested, this process produces 400 million pounds of para-xylene per annum from our chosen input, sugar cane molasses. In spite of the limited information available on cutting-edge technology, we believe the following process accurately estimates the costs and challenges associated with the renewable production of para-xylene, as well as identifies the key drivers of feasibility and profitability for further investigation.

Based on para-xylene and benzene selling prices of $0.83 and $0.45 per pound, respectively, and a purchase cost of $0.03 per pound for sugar cane molasses, as well as further considerations contained within this report, we believe that the renewable production of para-xylene is not profitable, and recommend against construction of the process. However, we recommend further research into yields obtainable in aqueous phase reforming and in condensation, as well as the cost to manufacture zeolite or similarly-capable catalysts; both will profoundly alter our economic analysis and may enable this project to offer significant returns to the investor.

Sincerely,

________________________  ______________________  ______________________  ______________________

Eric Castillo          Tyler Ernst          Corey Lerch           Parker Winchester
## Contents

Contents .................................................................................................................. 4

I. INTRODUCTION ............................................................................................................ 13

Abstract .................................................................................................................. 13

Process Overview .................................................................................................. 14

Input Analysis ........................................................................................................ 15

   Phase One: Screening by Cost Estimation .......................................................... 16

   Phase Two: In-Depth Screening ............................................................................ 18

II. MARKET & COMPETITIVE ANALYSIS .................................................................. 21

Porter’s Five Forces .................................................................................................. 21

   Bargaining power of suppliers ........................................................................... 21

   Bargaining power of customers .......................................................................... 22

   Threat of new entrants ....................................................................................... 22

   The Threat of Substitute products ...................................................................... 23

   Competitive Rivalry .......................................................................................... 23

SWOT Analysis .......................................................................................................... 24

   Strengths ............................................................................................................. 24

   Weaknesses ......................................................................................................... 24

   Opportunities ...................................................................................................... 25

   Threats .................................................................................................................. 26

III. OVERVIEW, FLOWSHEETS, and MATERIAL BALANCES .................................. 29

Overview ................................................................................................................ 29

Section 000: Input Storage & Clarification ............................................................... 31

Section 100: Hydrolysis ............................................................................................ 34

   Pre-hydrolysis .................................................................................................... 34

   Catalyst .............................................................................................................. 34

   Hydrolysis ......................................................................................................... 35

Section 200: Hydrogenation ...................................................................................... 40

   Pre-Hydrogenation ............................................................................................ 40

   Catalyst .............................................................................................................. 40

   Hydrogenation .................................................................................................. 41

Section 300: Aqueous Phase Reforming ................................................................. 48
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>000</td>
<td>Input Storage &amp; Clarification</td>
<td>93</td>
</tr>
<tr>
<td></td>
<td>Storage Tanks</td>
<td>93</td>
</tr>
<tr>
<td></td>
<td>Pumps</td>
<td>93</td>
</tr>
<tr>
<td></td>
<td>Other Equipment</td>
<td>93</td>
</tr>
<tr>
<td>100</td>
<td>Hydrolysis</td>
<td>94</td>
</tr>
<tr>
<td></td>
<td>Pumps</td>
<td>94</td>
</tr>
<tr>
<td></td>
<td>Heat Exchangers</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td>Reactors</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td>Catalyst</td>
<td>95</td>
</tr>
<tr>
<td>200</td>
<td>Hydrogenation</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>Pumps</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>Heat Exchangers</td>
<td>97</td>
</tr>
<tr>
<td></td>
<td>Reactors</td>
<td>98</td>
</tr>
<tr>
<td></td>
<td>Catalyst</td>
<td>98</td>
</tr>
<tr>
<td>300</td>
<td>Aqueous Phase Reforming</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Pumps</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Heat Exchangers</td>
<td>101</td>
</tr>
<tr>
<td></td>
<td>Reactors</td>
<td>102</td>
</tr>
<tr>
<td></td>
<td>Separators</td>
<td>103</td>
</tr>
<tr>
<td></td>
<td>Compressors</td>
<td>104</td>
</tr>
<tr>
<td></td>
<td>Catalyst</td>
<td>104</td>
</tr>
<tr>
<td>400</td>
<td>Condensation</td>
<td>105</td>
</tr>
<tr>
<td></td>
<td>Pumps</td>
<td>105</td>
</tr>
<tr>
<td></td>
<td>Heat Exchangers</td>
<td>106</td>
</tr>
<tr>
<td></td>
<td>Reactors</td>
<td>108</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>500</td>
<td>Separations</td>
<td>110</td>
</tr>
<tr>
<td>P-500</td>
<td></td>
<td>110</td>
</tr>
<tr>
<td>600</td>
<td>Transalkylation</td>
<td>116</td>
</tr>
<tr>
<td>Pumps</td>
<td></td>
<td>116</td>
</tr>
<tr>
<td>Heat Exchangers</td>
<td></td>
<td>116</td>
</tr>
<tr>
<td>Reactors</td>
<td></td>
<td>117</td>
</tr>
<tr>
<td>700</td>
<td>Furnace &amp; Heating Cycles</td>
<td>118</td>
</tr>
<tr>
<td>Storage Tanks</td>
<td></td>
<td>118</td>
</tr>
<tr>
<td>Furnaces</td>
<td></td>
<td>119</td>
</tr>
<tr>
<td>Pumps</td>
<td></td>
<td>120</td>
</tr>
<tr>
<td>VI. SPECIFICATION SHEETS</td>
<td></td>
<td>125</td>
</tr>
<tr>
<td>VII. OTHER CONSIDERATIONS</td>
<td></td>
<td>183</td>
</tr>
<tr>
<td>Alternate Design Considerations</td>
<td></td>
<td>183</td>
</tr>
<tr>
<td>Removal of Aqueous Phase Reforming Section</td>
<td></td>
<td>183</td>
</tr>
<tr>
<td>Woody Biomass with Three-Phase Hot Water Extraction</td>
<td></td>
<td>183</td>
</tr>
<tr>
<td>Alternative Separation Scheme</td>
<td></td>
<td>185</td>
</tr>
<tr>
<td>Invertase-Catalyzed Sucrose Hydrolysis</td>
<td></td>
<td>187</td>
</tr>
<tr>
<td>Plant Startup</td>
<td></td>
<td>187</td>
</tr>
<tr>
<td>Environmental Considerations</td>
<td></td>
<td>188</td>
</tr>
<tr>
<td>Process Control</td>
<td></td>
<td>189</td>
</tr>
<tr>
<td>Section 100: Hydrolysis</td>
<td></td>
<td>189</td>
</tr>
<tr>
<td>Section 200: Hydrogenation</td>
<td></td>
<td>190</td>
</tr>
<tr>
<td>Section 300: Aqueous Phase Reforming</td>
<td></td>
<td>191</td>
</tr>
<tr>
<td>Section 400: Condensation</td>
<td></td>
<td>192</td>
</tr>
<tr>
<td>Section 500: Separation</td>
<td></td>
<td>192</td>
</tr>
<tr>
<td>Section 600: Transalkylation</td>
<td></td>
<td>193</td>
</tr>
<tr>
<td>Section 700: Furnace</td>
<td></td>
<td>194</td>
</tr>
<tr>
<td>Safety Considerations</td>
<td></td>
<td>194</td>
</tr>
<tr>
<td>VIII. PROCESS ECONOMICS</td>
<td></td>
<td>197</td>
</tr>
</tbody>
</table>
The crystallizer must remove 2,293,914.1 BTU per hour in order to chill the mixed xylenes to -22 °F from 60°F. Additionally, the crystallizer requires 69.347 BTU per pound p-xylene to account for the latent heat of crystallization, and with 50,321.7 pounds per hour p-xylene product. This means 3,489,658.93 BTU per hour is required to crystallize the p-xylene. Therefore a total of 5,783,573.03 BTU per hour of refrigeration is used by the crystallizer unit.

At a cost of $10.867 per million BTU of heat removed for -90°F refrigerant, the total crystallization utilities are $62.85 per hour, or about $500,000 per year.
Appendix E: Sample ASPEN Block Reports

BLOCK:  CMP-300  MODEL: MCOMPR ................................................................. 464
BLOCK:  DC-500 .............................................................................................. 466
BLOCK:  F-300 ................................................................................................ 483
BLOCK:  HX-100 .............................................................................................. 484
BLOCK:  P-000 ................................................................................................ 487
BLOCK:  R-100 ................................................................................................ 487

Appendix D: Materials

Dowtherm A Specifications ................................................................. 263
Molten Salts Specifications (Kearney, 2002) ............................................ 265
Material Safety Data Sheets ................................................................. 267

Appendix C: Patents

US2011/0257448-A1 ................................................................................. 248
US5730837 .................................................................................................. 253
US6323381 ................................................................................................ 257
WO/2007075476-A2 .................................................................................. 260

Appendix B: Block Reports

SC-700: Combustion Energy Availability .................................................. 236
SC-701: Sizing and Pricing for Heating Fluid Storage Vessels ................. 237
SC-702: Pricing of Fired Heaters ............................................................... 237
SC-U00: Heating Fluid Requirements and Costs ....................................... 238
SC-U01: Utility Savings Calculations ......................................................... 238
SC-C00 ........................................................................................................ 239
SC-C01 ........................................................................................................ 240
SC-C02 ........................................................................................................ 240
SC-C03 ........................................................................................................ 241
SC-C04 ........................................................................................................ 241
DC-500 Concentration Profile ................................................................. 242
DC-500 Real Tray Efficiency Calculations ................................................. 243
DC-501 McCabe Thiele Analysis .............................................................. 244
DC-502 McCabe Thiele Analysis .............................................................. 245
DC-503 McCabe Thiele Analysis .............................................................. 246
SC-600: Sizing of HX-600 ........................................................................ 247

Appendix C: Patents

US2011/0257448-A1 ................................................................................. 248
US5730837 .................................................................................................. 253
US6323381 ................................................................................................ 257
WO/2007075476-A2 .................................................................................. 260
Section I
Introduction
I. INTRODUCTION

Abstract

This report details a process designed to renewably produce 400 million pounds of para-xylene per year from corn dry grind, sugar cane molasses (SCM), or woody biomass while minimizing water use. The para-xylene should be suitable for the production of polymers and plastics, and should be economical and green. All three feedstocks are equally suitable for the process and available for use.

The process is designed for SCM and consumes a total feed of 9.35 billion pounds of molasses per year. Corn dry grind is simply too expensive, and biomass, while cheaper per pound, imposes too many additional pre-processing costs. The molasses first undergoes hydrolysis then hydrogenation, followed by condensation and separation involving distillation and crystallization. Transalkylation and aqueous phase reforming are also employed to boost yield and create a self-contained process.

Several key assumptions are inherent in this process’s design. First, all reactor yields come directly from specific examples in the literature. Second, results found in the patents for glycerol were assumed valid for sorbitol as well, since not all patents used the same materials for their examples. Third, the economic analysis assumes that raw materials for catalyst manufacture can be purchased in bulk for a quarter of the price for small quantities. This assumption was suggested by Dr. Fabiano.

Based on these assumptions, the process designed herein meets the desired non-financial criteria, but results in an investor’s rate of return of negative 2.90% and a net present value of negative $196 million. However, further research into the catalyst or reactor yields could easily allow the process to break even or offer an attractive return.
Process Overview

This process aims to produce 400 million pounds of para-xylene per year from woody biomass, corn dry grind, or sugar cane juice, and must be both environmentally friendly and water-conserving. The para-xylene must be suitable for use in the manufacture of polymeric fibers and plastics such as polyethylene terephthalate (PET).

Para-xylene is a critical component in the manufacture of PET, used in high quantities to produce fibers, bottles, and other synthetic plastics and polymers. The market for para-xylene has grown by five to ten percent annually over the last several years, and is predicted to continue doing so in the near future. Current para-xylene production consumes valuable and non-renewable hydrocarbon-based feed materials. As demand continues to rise and these resources continue to dwindle, consumers of para-xylene foresee an unwelcome increase in the monetary and societal cost of these processes, and are actively seeking renewable alternatives as part of their environmental initiatives. Other than its more desirable environmental impact, renewably-produced para-xylene is indistinguishable from conventionally-produced para-xylene when used by the consumer. While somewhat small in comparison to the large para-xylene producers, 400 million pounds per year would signify a key first step towards renewable production in this market. There are currently no commercially operational plants that renewably produce para-xylene.

The process contained herein aims to renewably produce 400 million pounds of para-xylene per year. In addition to producing the specified quantity of para-xylene, the process also generates additional water which is recovered and reused. Significant quantities of benzene are also produced, which can be sold off for use in other industries. The process was designed to produce as many of its own materials as possible, including the water recovered from the process and the hydrogen generated in the aqueous phase reforming. The process also takes advantage of recycle loops to
ensure high levels of conversion and recovery, but does so without the use of additional costly units and equipment, aside from the increase in size associated with recycle streams. Only the sugar cane juice must be purchased externally, and is available from sugar cane ethanol facilities already acquired by the investigating company.

Molasses was chosen over corn dry grind due to its superior upfront cost, and over woody biomass due to the pre-processing costs bypassed by using a material already composed of sucrose. The process’s demand for molasses will, however, be significant enough to be noticed by the molasses market at large, and will likely affect the equilibrium market price.

Information used to design individual blocks within the process comes from patents and other relevant literature. The design adhered strictly to specific examples within the literature in order to ensure a conservative and accurate assessment of the process’s feasibility. Most notably, yields from the aqueous phase reforming, condensation, and transalkylation reactors were constrained to remain consistent with examples found in patents. However, the number of specific examples was limited, and as a result the process hinges on several key parameters, such as catalyst prices and reactor yields, that must be further investigated to provide a final assessment of the project’s economic viability. Based on the information available at present, the process is not profitable, but a small and reasonable shift in any one of several key parameters, discussed in greater detail in the report, would dramatically alter this prognosis.

Input Analysis

A major component of the design objectives is the identification of the optimal raw material input for a green para-xylene production process. The company commissioning this design recently acquired corn dry-grind (Nebraska) and sugar-cane ethanol (São Paolo) facilities; additionally, the company is negotiating a woody biomass supply from Washington. In order to determine the optimal raw material input(s), a sequential analysis was performed. In phase one of the analysis, corn dry-
grind outputs were eliminated on the basis of cost; in phase two, sugar cane molasses (SCM) won out as the optimal input on the basis of cost and availability.

**Phase One: Screening by Cost Estimation**

*Corn Dry-Grind*

The production of ethanol requires that whole grain corn be ground into a powder, which enters aqueous slurry and is fermented. The waste from this process is called the whole stillage. Whole stillage undergoes phase separation, the solids portion of which is called wet distillers’ grains with solubles (WDGS). WDGS is frequently dried and sold as dried distillers’ grains with solubles (DDGS). DDGS is used as livestock feed, and the drying process helps extend its shelf life. It was assumed that both WDGS and DDGS would be available to the designed facility. Information on these inputs is available in Figure 1, but the important takeaway is that DDGS and WDGS contain 29.4% and 33.4% sugar (glucan and xylan), respectively (Kim, 2008).

*Figure 1*

Suppliers for both WDGS and DDGS were located, which showed Midwest market prices to be ~$90/ton and ~$225/ton, respectively (Horner, 2012). The Scoular Company is an exemplary supplier due to its theoretical proximity (headquartered in Kansas), its scale (376M bushels and $4.9B sales annually), and its product line (i.e., availability of WDGS in addition to the more
common DDGS) (Scoular). These factors were advantageous because Scoular represents likely the lowest transportation costs and an accurate reflection of market-wide prices.

**Sugar-Cane By-products**

The primary material of interest in the sugar-cane ethanol process is a raw cane juice and molasses mixture, which is typically used as the primary feedstock after the sugarcane is initially processed. Unfortunately, market information for the molasses mixture is not easily attainable. Since it is a feedstock produced *in situ*, it does not have a secondary market like DGS. That said, Gopal (2009) identified a rough market price of Brazilian sugar cane molasses at ~$60/ton. The same article notes higher real and opportunity costs for cane juice - “molasses has a significantly lower opportunity cost than raw cane juice” – so molasses became the sole focus of the evaluation henceforth. Note that the standard molasses concentration of total reducible sugars (TRS) was initially taken to be 50%. Finally, note that world production is estimated at 61.7 million tons, with roughly 25% of the world’s supply produced in Brazil, the proposed location of this facility (Licht, 2011).

**Woody Biomass**

The source of woody biomass identified in the project is located in the state of Washington. The description notes forest-thinning, mill residue, and land-clearing debris would be available. In a 2005 report by funded by the state government, Biomass Inventory and Bioenergy Assessment, the supply of such biomass in WA is noted as 6.3 million tons (Frear). Furthermore, in a 2000 study, it was estimated that mill residue could be delivered at a price of $30/ton (Antares Group). This latter figure is inflation-adjusted to $39.49 (CNM Group). It should be noted that this figure is optimistic since the original price quote was for a scale of 45 million tons, which significantly exceeds Washington’s total availability.
Initial Screening Results

Using the above figures, an initial screening solely on the basis of price permitted easy insight into the profitability ceiling of the proposed models. The comparative basis chosen was the maximum margin attainable. This is defined as the profit margin where the sole cost is input procurement (i.e., not factoring in the costs of equipment, transportation, utilities, etc.). This figure imposes a ceiling on process profitability and enabled the prioritization of research into the most theoretically profitable input materials. Woody biomass (WB), with a maximum margin of 93-97%, and SCM (at 94%) became the focus of effort. Note that WDS was found to be a viable alternative, but that it appears substantially more expensive than the other two inputs. DDGS was ruled out completely because it would cost ~3-10x more than the other inputs.

Phase Two: In-Depth Screening

The second phase of the input screening involved a closer look at getting raw materials to usable process inputs. It was quickly conclusive that SCM was favorable. Given that both substances are produced in enormous quantities, it was necessary to distinguish between them along another dimension - the question became one of whether the $20/ton savings from using biomass was worth the added enzymatic or acid-catalyzed processing to convert cellulose to glucose. Enzymes were quickly ruled out on the basis of cost and the necessity of a batch process. Acid-catalyzed processing was appealing, but ultimately, the route from SCM to glucose appeared both simpler and easier -- largely just adding water and decanting --, well in excess of the $20 savings per ton.
Section I: Introduction
Section II
Market & Competitive Analysis
II. MARKET & COMPETITIVE ANALYSIS

Porter’s Five Forces

The Porter’s Five Forces framework, developed by Michael Porter of the Harvard Business School in 1989, provides a framework to identify and evaluate less tangible aspects of a prospective market. The framework allows the user to evaluate attractiveness of the market based on (1) the bargaining power of suppliers, (2) the bargaining power of customers, (3) the threat of new entrants (4) the threat of substitute products, and (5) competitive rivalry within the industry. Based on the prevalence of each of these forces, prospective entrants can better evaluate a project’s potential.

Bargaining power of suppliers

The molasses used as feedstock is the only material that must be purchased externally. Fermentation processes use molasses to produce baker’s and brewer’s yeast, citric acid, industrial alcohol, monosodium glutamate, and lysine. In addition, many industries, in particular agricultural feed manufacturing, use molasses for its binding properties (DMH Website). The presence of these additional buyers implies a high bargaining power among suppliers. Furthermore, suppliers are likely to lower production in response to a predicted surplus (DMH MB), which would further increase suppliers’ leverage.

However, Cuba recently replaced its Ministry of Sugar with 13 separate state enterprises. The number of active sugar mills fell from 61 to 56, but overall bargaining power will fall without the ability to negotiate collectively. In addition, Beet molasses prices in eastern Europe have fallen dramatically (DMH MB), which will decrease the demand for cane molasses and further reduce suppliers’ bargaining power. Overall, bargaining power of suppliers, while moderately high, should decay somewhat in the near future.
**Bargaining power of customers**

Xylene and particularly para-xylene are already produced in high volumes within the United States. It serves as a solvent in the printing, rubber, and leather industries, as well as a cleaning agent, a thinner for paint, and a component of many varnishes. Gasoline also contains para-xylene in small quantities. Most importantly, producers of synthetic fibers and plastics rely on para-xylene to manufacture polyester and related compounds like polyethylene terephthalate (PET); plastic bottle production alone represents 98% of global para-xylene consumption (Habeck 1995). These industries are dominated by large companies, such as Koch industries, who can use their size to exert high bargaining power.

In addition, supplies of para-xylene more than satisfy demand. Worldwide production capacity exceeded demand by over 4.5 million metric tons, meaning that average capacity utilization resides below 80%. In the short term, this likely counteracts any disadvantages in bargaining power that plague para-xylene customers. However, in the long term, the demand for para-xylene is expected to continue growing at 7% per annum, which should eliminate this excess capacity (Primary Information Services). Overall, the bargaining power of customers is high, but should decay steadily in the future.

**Threat of new entrants**

Demanders of para-xylene are actively encouraging a fiercely competitive para-xylene market inhabited by numerous new entrants, particularly those focused on renewable production. Most recently, Coca-cola, whose bottle manufacturing represents a significant fraction of annual para-xylene demand, recently invested in partnerships with three separate companies developing renewable para-xylene or substitute production processes: Gevo, Virent, and Avantium. In fact, Virent’s technology served as the basis for this process’s design. Pepsi, Coca-Cola’s chief competitor, responded with in-house development of their own renewable para-xylene production process. Both Coca-Cola and Pepsi expect to use these processes commercially by 2015 (Lane
Section II: Market & Competitive Analysis

2011). This means that even as demand continues to grow, new entrants will maintain a fierce level of competition in the para-xylene market.

The Threat of Substitute products
Para-xylene and its enabled polymer, polyethylene terephthalate (PET), have long served the markets mentioned under “Bargaining Power of Customers.” However, Avantium, a company that recently partnered with both Coca-Cola and Danone Research, is currently developing what they claim to be a viable alternative, polyethylene furanoate (PEF) using its patented YXY (“icksy”) catalyst technology. Independent studies by the Copernicus Institute at Utrecht University showed that PEF has a 50-60% lower carbon footprint that oil-based PET, and Avantium further claims that PEF is both lighter and more thermally resistant than PET (Danone, 2012).

However, the process has not yet proven industrially viable. In addition, a renewable para-xylene production process would mitigate or eliminate the carbon footprint advantages of PEF, dramatically lowering the incentive for bottle manufactures to invest in a transition to PEF. Because of these mitigating factors, the threat of substitutes is moderate.

Competitive Rivalry
Due to economies of scale, as well as consumer tendencies to require high quantities of para-xylene, the market is dominated by a significant number of high-capacity firms that operate internationally. Some, such as Invsita, a subsidiary previously owned by DuPont and recently purchased by Koch Industries, are vertically integrated, and provide their own demand for para-xylene in the form of polymers and polymer intermediates used in surfaces, materials, resins, and apparel (Koch, 2012). Others, such as Reliance Industries, have a more diversified portfolio. These companies produce para-xylene in quantities far exceeding the 200,000 tons of this process’s design (Reliance Industries is the 5th largest at 1.86 million tons) (Reliance, 2012). With so many large competitors, competitive rivalry is expected to be high.
SWOT Analysis

SWOT stands for Strengths, Weaknesses, Opportunities, and Threats. After analyzing the state of Porter’s Five Forces above, a SWOT framework enables the user to contextualize the information, draw conclusions, and make decisions.

Strengths
The first strength of this process is renewability. Para-xylene is not a new chemical, and the market has many large and well-established players. However, in the new age of environmental responsibility, the largest consumers of para-xylene are search for, and willing to invest heavily in, renewable alternatives to their current supplies. This creates competitive advantage over large incumbents in the market.

Second, the process was designed to take advantage of excess benzene produced during condensation and transalkylation. Although not quite as lucrative as para-xylene, benzene is still a valuable chemical. In addition to the additional profit offered by this benzene on a regular basis, it provides greater financial stability for the process. Both para-xylene and benzene demand and prices have been historically volatile, but have not always followed one another. As such, should the price of para-xylene drop unexpectedly, the process will still generate revenue from the sale of benzene.

Third, the para-xylene market in general is growing at an expected rate of 7% per annum. At this rate, there should be sufficient demand for para-xylene in general to sustain the process. Furthermore, if the market continues to grow, this process could be expanded or replicated elsewhere in order to establish a stronger foothold in the market at large.

Weaknesses
First, the process is dependent on molasses as a feedstock. Because suppliers of molasses are expected to exert a large amount of bargaining power in the near future, they could easily negotiate higher prices in response to an increase in demand, which would have a direct impact on the
Section II: Market & Competitive Analysis

process’s profitability. Unfortunately, the process’s molasses requirements represent a significant fraction of molasses production in Brazil, essentially ensuring that prices will rise.

Second, the dominance of large and established para-xylene suppliers implies that this process will have to compete fiercely for customers, as well as accept market prices as given. Should the operating or materials costs rise for this particular process, it will be difficult to negotiate higher prices when larger competitors continue to sell at historical levels.

Third, the current excess para-xylene production capacity suggests that finding customers immediately upon market entry will be difficult. Most likely, the process will have to cater to smaller niche buyers, which will increase organizational costs and directly affect profitability.

Opportunities

First and foremost, the largest consumers of para-xylene are actively searching for a renewable source of para-xylene. These buyers are large. They are adverse to change in general, and place a high value on mitigating risk. As already demonstrated by Virent, Gevo, and Avantium, these companies are willing to subsidize further research. In addition, whichever company is first to market will capture a large customer, who will have little incentive to switch to any new entrant without a significantly superior value proposition.

Second, many industries, both those mentioned in the “Bargaining Power of Customers,” and others, that could either begin using or make greater use of para-xylene are largely overlooked by the large players in the market. A smaller plant, such as this one, could better serve these smaller customers in a smaller, more profitable niche market while simultaneously contributing to increased total demand.

Third, although molasses prices are predicted to rise in response to this new para-xylene production process, the current slump in demand for cane molasses provides an opportunity to
Castillo, Ernst, Lerch, Winchester
mitigate these rises. Molasses suppliers will dislike falling prices, and should be more willing to enter into long-term contracts at the current market price in order to avoid short-term losses.

**Threats**

First, Virent and Gevo are already developing similar processes for the renewable production of para-xylene. If either succeeds and enters the market first, they are likely to capture most or all of the demand for renewable para-xylene. This will leave later entrant to either battle to steal market share or compete with non-renewable suppliers for customers. Either represents a challenge for late entrants to operate at full-capacity.

Second, Avantium’s prototype process for PEF threatens to decrease demand for para-xylene overall. This will have the direct effect of lowering the market price of para-xylene. Indirectly, many of Porter’s Five Forces are currently unfavorable for a new entry, but are expected to improve as a result of steady increase in demand. If PEF proves viable and superior to PET, these conditions will remain unfavorable and make profitable operation in the market difficult.
Section III
Process Overview, Flowsheets, & Material Balances
III. Overview, Flowsheets, and Material Balances

Overview

The goal of this process is to produce para-xylene from sugar cane molasses. From storage, molasses is pumped to the clarifying section in which ash and other impurities are removed to form a sucrose and water solution. The sucrose is then hydrolyzed to form glucose and fructose. The glucose and fructose are then hydrogenated to form sorbitol. Sorbitol is used in the aqueous phase reforming to produce hydrogen, which is consumed in the hydrogenation reaction. The majority of the sorbitol is reacted in the condensation section to form aromatics and other organic compounds. These compounds are then separated through distillation. Certain alkanes and aromatics are then reacted in the transalkylation section through which additional para-xylene is formed, which is then sent back to the separation section. In the separation section, para-xylene is separated from similar compounds through crystallization to yield the final product.
Section III: Process Overview, Flowsheets, & Material Balances

Section 000: Input Storage & Clarification

Molasses is produced only nine months per year, which means that storage to maintain output levels throughout the three dry months is a key process consideration. This section details the storage of molasses, which requires 15 cone-roof tanks. One-third of these tanks will be in active use at any given time during the molasses season. The other two-thirds will be used to build up molasses supply throughout the year so that production can continue for the 92 days without raw material supply.

Molasses is a raw material produced from sugar cane and has many impurities in it such as ash and various minerals and carbohydrates besides the desired sugars, sucrose, glucose, and fructose. In order to remove these impurities and produce a sugar and water stream to be fed into the hydrolysis section, the molasses must undergo clarification. Molasses is first diluted with water in a heated continuously stirred mixer. Phosphoric acid and sodium hydroxide are added to precipitate impurities. Once diluted, the mixture is fed to a large concrete clarifying vessel. This allows the precipitated material to settle on the bottom of the clarifier, where it is scraped away by a rotating rake and leaves the clarifier as a sludge. The liquid overflow from the clarifier is pumped through a rotary drum filter where impurities are further removed from the mixture. Excess water is then evaporated to form a 50% sugar by mass solution, which is then pumped to the hydrolysis section.

Since the project description states that the company has recently acquired “sugar-cane ethanol facilities” in Brazil, it is a reasonable assumption that the facilities are capable of molasses clarification and processing. Because of this assumption, we focused on the aspects of the process downstream of the conversion of raw molasses into a sugar and water solution.

However, a qualitative analysis of molasses clarification was examined and conservative estimates for the equipment and materials required were performed.
For each pound of molasses fed into the clarification process, .003 pounds of phosphoric acid and .004 pounds of sodium hydroxide would be required. Additionally, .00006 pounds of flocculant would be necessary. For our process, 1,183,104 pounds per hour of molasses are required. At a cost of $850 per ton of phosphoric acid, $12 million per year would be spent on phosphoric acid. At a cost of $500 per ton, $9 million per year would go to sodium hydroxide. Flocculant would cost only $295,000 per year.

A concrete clarifier with settling area of 88,258 square feet would cost $1,255,988 to purchase. The rotary drum filter, removing 1500 pounds of filtrate per day per square foot, would have to have an area of 115 square feet and would cost $130,000. In addition to this, an evaporator would likely be necessary to evaporate some of the water to turn the dilute sugar solution into a 50% sugar solution.
Section 000: Input Storage & Clarification
Section 100: Hydrolysis

\[ C_{12}H_{22}O_{11} + H_2O \rightarrow 2 C_6H_{12}O_6 \]

The hydrolysis reaction converts sucrose and water into glucose. Sucrose is hydrolyzed by an HY faujasite zeolite catalyst, with a Si/Al ratio of 15. While sucrose hydrolysis could take place by itself in water, it would take years to fully hydrolyze. The catalyst is put in place to expedite the process to a much more reasonable reaction velocity. The product, glucose, is the necessary feed materials for the hydrogenation reactor needed to generate sorbitol.

The hydrolysis reaction process involves a splitter (SPT-100), six pumps (P-100, P-101, P-102, P-103, P-104, and P-105), three heat exchangers (HX-100, HX-101, and HX-102), and three fixed bed reactors (R-100, R-101, and R-102) to convert sucrose and water to glucose.

Pre-hydrolysis

The system input is fed into a splitter to make three identical streams and fed into the first three pumps (P-100, P-101, and P-102). The pumps are used to begin the flow of material throughout the process and make up for the frictional losses caused by the pipes. These pumps, feed the three heat exchangers (HX-100, HX-101, and HX-102). The heat exchangers are used to heat up the reactor feed streams to 100°C, while simultaneously cooling the condensation product stream.

Catalyst

The HY faujasite catalyst can easily made by feeding H4SiO4 and NaAlO2 in a ratio of about 12 to 1 in the presence of NaOH and excess water. Faujasite crystals are formed through the use of steam aging HY crystals at 500°C for about 2 hours. To adjust the Si/Al ratio, after the steam aging, aqueous (NH4)2SiF6 is used until the Si/Al ratio is 15. The catalyst deactivation is estimated to be 13.9 g catalyst/lbmol sucrose fed, based on the deactivation rate of a similar catalyst, however the deactivation rate may actually be lower than estimated. The reason for the possibility of lower deactivation is evidenced by the claim that by running the reactor for 7 days, at a low flow, rate no
deactivation was observed. The catalyst can also easily be regenerated through a thermal treatment, in which hot air at 500°C is passed through the catalyst for 2 hours, when it has lost significant activity a limited number of times.

**Hydrolysis**

Once the streams are heated up they are fed into the three reactors (R-100, R-101, and R-102). The reactors are typical industrial fixed bed reactors. They are essentially a series of tubes, filled with catalyst, in parallel. The tubes are laid out in such a way as to look similar to a shell and tube heat exchanger with many tubes. The reactors used for this process have over 10000 tubes per reactor. All three reactors operate at atmospheric pressure and 100°C and convert 100% of the sucrose to glucose. Once the reaction has taken place the three product streams are fed into the other three pumps to raise their pressure to 80 bar, after which they are mixed and fed into the next section.

These reactors were based off of examples found in the literature, in particular Moreau (1999). To hydrolyze sucrose, an approximately 600 g/l solution of sucrose is fed through a tubular reactor charged with the HY faujasite catalyst. The fixed bed reactor is held at 100°C. It was observed that approximately 99.9% of all sucrose fed into the reactor was converted to glucose.
Section 100: Hydrolysis
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>618205</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>618205</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Dowtherma</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Flow (lbmol/hr)</td>
<td>36122</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
<td>12041</td>
</tr>
<tr>
<td>Total Flow (lb/hr)</td>
<td>1236410</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
<td>412136</td>
</tr>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>16714</td>
<td>5571</td>
<td>5571</td>
<td>5571</td>
<td>5571</td>
<td>5571</td>
<td>5571</td>
<td>5571</td>
<td>5953</td>
<td>5953</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>77.00</td>
<td>77.00</td>
<td>77.00</td>
<td>77.00</td>
<td>77.04</td>
<td>77.04</td>
<td>77.04</td>
<td>77.04</td>
<td>212.00</td>
<td>212.00</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>40.41</td>
<td>41.15</td>
<td>41.15</td>
<td>40.41</td>
<td>41.15</td>
<td>41.15</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
### Hydrolysis Stream Report (2 of 3)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>41138</td>
<td>13712</td>
<td>13713</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>763</td>
<td>254</td>
<td>254</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>85</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6059</td>
<td>2020</td>
<td>2020</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>23225</td>
<td>7741</td>
<td>7742</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>32312</td>
<td>10771</td>
<td>10771</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>195221</td>
<td>195221</td>
<td>195221</td>
<td>195221</td>
<td>195221</td>
<td>195221</td>
<td>585662</td>
<td>792890</td>
<td>264294</td>
<td>264302</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>389</td>
<td>130</td>
<td>130</td>
</tr>
<tr>
<td>Glucose</td>
<td>216916</td>
<td>216916</td>
<td>216916</td>
<td>216916</td>
<td>216916</td>
<td>216916</td>
<td>650747</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>424</td>
<td>141</td>
<td>141</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>9087</td>
<td>3029</td>
<td>3029</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2019</td>
<td>673</td>
<td>673</td>
</tr>
<tr>
<td>Napthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>20195</td>
<td>6732</td>
<td>6732</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>20195</td>
<td>6732</td>
<td>6732</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>30293</td>
<td>10098</td>
<td>10098</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>7068</td>
<td>2356</td>
<td>2356</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>972</td>
<td>324</td>
<td>324</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2934</td>
<td>978</td>
<td>978</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>4081</td>
<td>1360</td>
<td>1361</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>893</td>
<td>298</td>
<td>298</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

<p>| Total Flow (lbmol/hr)   | 12040 | 12040 | 12040 | 12040 | 12040 | 36121 | 46295 | 15432 | 15432 |
| Total Flow (lb/hr)      | 412136| 412136| 412136| 412136| 412136| 1236410| 995023| 331671| 331681|
| Total Flow (cuft/hr)    | 5745  | 5745  | 5745  | 5753  | 5753  | 17259 | 822002| 273998| 274006|
| Temperature (°F)        | 212.00| 212.00| 212.00| 214.16| 214.16| 214.16| 214.16| 698.00| 698.00|
| Pressure (psia)         | 14.70 | 14.70 | 14.70 | 1181.70| 1181.70| 1181.70| 1181.70| 639.70| 639.70|
| Vapor Fraction          | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 1.00  | 1.00  | 1.00  |</p>
<table>
<thead>
<tr>
<th>Mass Flow (lb/hr)</th>
<th>S-419</th>
<th>S-420</th>
<th>S-421</th>
<th>S-422</th>
<th>S-423</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>13712</td>
<td>13712</td>
<td>13712</td>
<td>13713</td>
<td>41138</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>254</td>
<td>254</td>
<td>254</td>
<td>254</td>
<td>763</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>28</td>
<td>28</td>
<td>28</td>
<td>28</td>
<td>85</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>2020</td>
<td>2020</td>
<td>2020</td>
<td>2020</td>
<td>6059</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>7741</td>
<td>7741</td>
<td>7741</td>
<td>7742</td>
<td>23225</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>10771</td>
<td>10771</td>
<td>10771</td>
<td>10771</td>
<td>32312</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>264294</td>
<td>264294</td>
<td>264294</td>
<td>264302</td>
<td>792890</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>130</td>
<td>130</td>
<td>130</td>
<td>130</td>
<td>389</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>141</td>
<td>141</td>
<td>141</td>
<td>141</td>
<td>424</td>
</tr>
<tr>
<td>Toluene</td>
<td>3029</td>
<td>3029</td>
<td>3029</td>
<td>3029</td>
<td>9087</td>
</tr>
<tr>
<td>Benzene</td>
<td>673</td>
<td>673</td>
<td>673</td>
<td>673</td>
<td>2019</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>6732</td>
<td>6732</td>
<td>6732</td>
<td>6732</td>
<td>20195</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>6732</td>
<td>6732</td>
<td>6732</td>
<td>6732</td>
<td>20195</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>10098</td>
<td>10098</td>
<td>10098</td>
<td>10098</td>
<td>30293</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>2356</td>
<td>2356</td>
<td>2356</td>
<td>2356</td>
<td>7068</td>
</tr>
<tr>
<td>1-Butene</td>
<td>324</td>
<td>324</td>
<td>324</td>
<td>324</td>
<td>972</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>978</td>
<td>978</td>
<td>978</td>
<td>978</td>
<td>2934</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>1360</td>
<td>1360</td>
<td>1360</td>
<td>1361</td>
<td>4081</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>298</td>
<td>298</td>
<td>298</td>
<td>298</td>
<td>893</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr) | 15432 | 15432 | 15432 | 15432 | 46295 |
| Total Flow (lb/hr)    | 331671| 331671| 331671| 331681| 995023|
| Total Flow (cuft/hr)  | 273998| 208888| 208889| 208897| 626674|
| Temperature (°F)      | 698.00| 505.98| 505.98| 505.98| 505.98|
| Pressure (psia)        | 639.70| 639.70| 639.70| 639.70| 639.70|
| Vapor Fraction        | 1.00  | 1.00  | 1.00  | 1.00  | 1.00  |
Section 200: Hydrogenation

\[ \text{C}_6\text{H}_{12}\text{O}_6 + \text{H}_2 \rightarrow \text{C}_6\text{H}_{14}\text{O}_6 \]

Hydrogenation reacts glucose with hydrogen gas and converts it to sorbitol. There are several ways to successfully convert glucose to sorbitol, in the presence of hydrogen and certain catalysts. Some combinations of catalysts, hydrogen pressures, and reactor temperature yield much better results in terms of overall conversion of glucose to sorbitol. Many of these variables were experimented with in search of the best results.

**Pre-Hydrogenation**

The hydrogenation process consists of a heat exchanger (HX-200), a splitter (SPT-200), twelve pumps (P-200, P-201, P-202, P-203, P-204, P-205, P-206, P-207, P-208, P-209, P-210, and P-211), and six trickle bed reactors (R-200, R-201, R-202, R-203, R-204, and R-205). HX-200 cools the streams to 100°C from the hydrolysis process before feeding them into the splitter, SPT-200 to create six identical streams. They are fed into the first six pumps (P-200, P-201, P-202, P-203, P-204, and P-205) to get them flowing into the six trickle bed reactors (R-200, R-201, R-202, R-203, R-204, and R-205) and make up for the frictional losses in the pipes. Hydrogen created in the APR process is fed into the reactors as well.

**Catalyst**

In typical glucose hydrogenation Ni used to be the preferred catalyst metal because of its high activity and low costs. Unfortunately Ni catalysts can leach and have their activity decreased rapidly and require possibly expensive separation processes to purify the product of the Ni particles. Ru catalysts however don’t suffer from the same drawbacks as Ni which makes it much more appealing as a commercial catalyst. The catalyst which yielded the best result for glucose hydrogenation was a Ru05Ai catalyst.
The Ru05Ai catalyst creation process would be prepared by the impregnation of Al2O3 with Ruthenium (III) Acetylacetonate. The Al2O3 is used as the support metal for the activation of the ruthenium. To begin the preparation of the catalyst 73 g Al2O3 is mixed with 150 ml of toluene and stirred for 15 minutes. Once the Al2O3/toluene slurry is prepared, 2.907 g Ruthenium (III) Acetylacetonate is dissolved in a separate 150 ml of toluene and this solution is added to the slurry. This new slurry is stirred for one hour while being swirled occasionally to homogenize it. The toluene is also left to evaporate at room temperature at this time. The catalyst is then heated in by a helium stream within four hours to 250°C and held at this temperature for two more hours. To reduce the catalyst it is heated to 350°C within one hour by a hydrogen stream and held at this temperature for three more hours. However based on the cost of buying of the raw materials needed and additional labor costs needed for creating the catalyst it was found to be much cheaper to purchase a catalyst that is believed to be similar from a supplier. Catalyst deactivation was assumed to be seven years because of Ruthenium’s use as a precious metal. It was also assumed that the catalyst could be sold back to the supplier for half of the purchase price.

Hydrogenation
There are two possible ways to do a glucose hydrogenation, either discontinuously or continuously. The discontinuous process involves feeding an autoclave with the feedstock and pressurizing it to 3 bar with hydrogen followed by increasing the temperature to its reaction temperature and then finally pressurizing the hydrogen to its desired pressure. This process unfortunately would take too much time and the continuous process is preferred in practice. The continuous process involves a trickle bed reactor. A typical reaction condition for this is a 40-wt% glucose solution with a large of excess of hydrogen gas at about 80 bar fed into a reactor at approximately 353K. A conversion of 99.9% of the glucose fed with selectivity to sorbitol of 99.0% was reported.
A trickle bed reactor is different from most conventional fixed bed reactors in that both the gas and liquid flow are pumped into the top of the reactor co-currently as opposed to having liquid flow downward and gas flow upward counter-currently. The hydrogenation reaction takes place at 353K and 80 bar and converts 100% of the glucose into sorbitol. The products streams are then fed into the other six pumps (P-206, P-207, P-208, P-209, P-210, and P-211) to get them flowing into the aqueous phase reforming and condensation processes and make up for the frictional losses caused by the reactor and pipes.
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>1284910</td>
<td>1284910</td>
<td>585662</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>650747</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90.00</td>
<td>119.17</td>
<td>214.16</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>14.70</td>
<td>14.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1181.70</td>
<td>1183.70</td>
<td>1183.70</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>------------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>97610</td>
<td>97610</td>
<td>97610</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
<td>97616</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>108458</td>
<td>108458</td>
<td>108458</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Flow (lbmol/hr)</td>
<td>6020</td>
<td>6020</td>
<td>6020</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
<td>6021</td>
</tr>
<tr>
<td>Total Flow (lb/hr)</td>
<td>206068</td>
<td>206068</td>
<td>206068</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
<td>207296</td>
</tr>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>2809</td>
<td>2809</td>
<td>2809</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
<td>2821</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>1183.70</td>
<td>1183.70</td>
<td>1183.70</td>
<td>1160.30</td>
<td>1160.30</td>
<td>1160.30</td>
<td>1160.30</td>
<td>1160.30</td>
<td>1160.30</td>
<td>1162.30</td>
<td>1162.30</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>------------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>109680</td>
<td>109680</td>
<td>109682</td>
<td>109680</td>
<td>658083</td>
<td>658083</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Par-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>97616</td>
<td>97616</td>
<td>97617</td>
<td>97616</td>
<td>585695</td>
<td>585695</td>
<td>585662</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>7369</td>
<td>1228</td>
<td>1228</td>
<td>1228</td>
<td></td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>650747</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr) | 6021 | 6021 | 6021 | 6021 | 36123 | 36123 | 36121 | 3656 | 609 | 609 | 609 |
| Total Flow (lb/hr)    | 207296 | 207296 | 207299 | 207296 | 1243780 | 1243780 | 1236410 | 7369 | 1228 | 1228 | 1228 |
| Total Flow (cuft/hr)  | 2821 | 2821 | 2821 | 2821 | 16928 | 16928 | 16852 | 22167 | 3693 | 3693 | 3693 |
| Temperature (°F)      | 175.73 | 175.73 | 175.73 | 175.73 | 175.74 | 175.74 | 175.80 | 175.73 | 175.73 | 175.73 | 175.73 |
| Pressure (psia)       | 1162.30 | 1162.30 | 1162.30 | 1162.30 | 1160.30 | 1160.30 | 1160.30 | 1164.30 | 1164.30 | 1164.30 | 1164.30 |
| Vapor Fraction        | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 1.00 | 1.00 | 1.00 |
## Section III: Process Overview, Flowsheets, & Material Balances

### Hydrogenation Stream Report (4 of 4)

<table>
<thead>
<tr>
<th>Mass Flow (lb/hr)</th>
<th>S-320</th>
<th>S-321</th>
<th>S-322</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1228</td>
<td>1231</td>
<td>1228</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Napthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### Economic Parameters

<table>
<thead>
<tr>
<th>Total Flow (lbmol/hr)</th>
<th>609</th>
<th>610</th>
<th>609</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Flow (lb/hr)</td>
<td>1228</td>
<td>1231</td>
<td>1228</td>
</tr>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>3693</td>
<td>3702</td>
<td>3693</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>1164.30</td>
<td>1164.30</td>
<td>1164.30</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>
Section 300: Aqueous Phase Reforming

Aqueous phase reforming (APR) is a novel technology for the catalytic conversion of oxygenated hydrocarbons into hydrogen, alkanes, and carbon dioxide (WO/2007075476-A2). It is a more sustainable alternative to fossil fuel reforming for processes that require an endogenous supply of hydrogen. In this process, APR can convert readily-available sugar alcohols into hydrogen, over a RhReCe catalyst, which is used to create sorbitol, a necessary intermediate in the production of para-xylene.

Although hydrogen is the goal output of this section, the light alkane by-products can be used to generate heat for other portions of the process. However, the data supplied in the patent detail conversion and output composition in lump sum “alkanes.” The relative break downs of alkanes in the final product is unknown. However, a sensitivity analysis of heats of combustion (Figure 2) showed that the actual composition of C1-C6 alkanes made little differential impact on the overall energy output (Pittam, 1972; SI Chemical Data Book).

Figure 2

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$\Delta C H^+$ [alkane]</th>
<th>Heat/mol RXN</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3) $C_6H_{14}O_6 \rightarrow 1.89 \text{ CO}_2 + 0.68 \text{ C}<em>4H</em>{14} + 2.21 \text{ H}_2\text{O}$</td>
<td>-4180 kJ/mol $^2$</td>
<td>-2842.4</td>
</tr>
<tr>
<td>(4) $C_6H_{14}O_6 \rightarrow 2.75 \text{ CO}_2 + 3.25 \text{ CH}_4 + 0.5 \text{ H}_2\text{O}$</td>
<td>-890.3 kJ/mol $^1$</td>
<td>-2893.5</td>
</tr>
<tr>
<td>Average:</td>
<td></td>
<td>-2867.9</td>
</tr>
</tbody>
</table>

Therefore, propane, which has a middling heat of combustion, was chosen as the sole alkane for all ASPEN calculations in this portion of the analysis.

The aqueous phase reforming process utilizes four heat exchangers (HX-300, HX-301, HX-302, and HX-303), three pumps (P-300, P-301, and P-302), two valves (VAL-300 and VAL 301), two flash separators (F-300 and F-301), a mixer (MIX-300), a pressure swing adsorption separator (SEP-300), a compressor (CMP-300) and a fixed bed reactor (R-300).
Catalyst

The catalyst presentation in the patent was presented independent of the operating conditions discussion. The most optimal conditions range from 150-300°C and from 10-50 bar. 182°C and 50 bar were selected as the duty-minimizing conditions, over which the specified conversions were assumed to apply. This is certainly a questionable assumption, but there was no other basis for condition selection available. The catalyst was made by adding 3.86g of Rhodium(III) Nitrate, 1.64g of Perrhenic acid, and 2.21g of Cerium(III) Nitrate hexahydrate to 12 ml of deionized water in the presence of titania modified carbon and dried overnight under a vacuum at 100°C. The titania modified carbon was created by adding 1.95g of Titanium n-butoxide to 12 ml of anhydrous isopropanol in the presence of 10g of activated carbon. However due to the high costs of Rhodium(III) Nitrate it was assumed that the metals were purchased at market price and could be sold back to the supplier after deactivation for half the purchase price to be regenerated. It was also assumed that because rhodium is a precious metal the deactivation would take place over 5 years.

Aqueous Phase Reforming

The patented technology (Cortright 2007) - assumed to be available for use in this plant - presents a range of operating conditions, inputs, and catalysts. Since sorbitol is a key component of the process, Example 31 from Table 7 was chosen for the design, as it maximizes hydrogen from a sorbitol input. Specifically, this embodiment converts a 50 wt% aqueous sorbitol solution to a gas that is 57 mol% hydrogen over a RhReCe catalyst in the presence of NaOH. Note that the patent is extraordinarily difficult to interpret, as the molar percentage of alkanes is uninterpretable on a mass basis, since the breakdown of alkanes is unknown. To overcome this, Excel solver was used to backout the actual yields for the process via a mole balance. The fixed bed reactor, R-300, is used to generate hydrogen, alkanes, and carbon dioxide from sorbitol.
Heat Exchange and Recovery

The first heat exchanger, HX-300, is used to cool the carbon dioxide, water, hydrogen and alkane stream from F-300 while simultaneously heating the new and recycled sorbitol mix stream from MIX-300. The second heat exchanger, HX-301, is used to heat the inlet sorbitol stream, fed to R-300, to 182°C, the reaction temperature by using the heat generated from the furnace. The third heat exchanger, HX-302, is used to cool the hydrogen stream coming from HX-400 to 353K the reaction temperature of the hydrogenation reaction. The fourth heat exchanger, HX-303, is used to cool the hydrogen, carbon dioxide, and alkane stream from HX-300 and is fed into F-301.

Pressurization and Depressurization

The first pump, P-300, is used to pump the new and recycled sorbitol mix stream from HX-300 to HX-301 and make up for any frictional losses. The second pump, P-301, is used to pump the recycled sorbitol from F-300 into MIX-300 and to make up for frictional losses. The third pump, P-302, is used to pump the new and recycled sorbitol mix from MIX-300 to HX-300 and to combat the frictional losses. The first valve, VAL-300, is used to decrease the pressure of the product stream mixed with the recyclable sorbitol from R-300. The second valve, VAL-301, is used to decrease the pressure of the hydrogen, carbon dioxide, water, and alkane stream from F-300. The compressor, CMP-300, is used to compress the hydrogen separated in SEP-300 to 80 bar to be fed to the hydrogenation process.

Separations

To recover hydrogen from the aqueous phase reforming reactor, the vapor product is separated using pressure swing adsorption (PSA). Hydrogen, carbon dioxide, water, and various light alkanes are flowed across several adsorption columns at 20 bar. The zeolites in the columns adsorb the polar components and carbon dioxide, while the hydrogen exits the column. Once the column becomes saturated, the outlet valve is shut off and a vacuum is pulled on the column, causing the polar components and carbon dioxide to desorb from the adsorbent and regenerate the
Section III: Process Overview, Flowsheets, & Material Balances

Once the column is regenerated, the cycle is repeated. Multiple adsorption columns are necessary to make optimal use of the compressor and vacuum, ensuring that at least one column is being fed vapor at any moment.

The first flash separator, F-300, is used to separate sorbitol from R-300 products so the sorbitol can be recycled. The second flash separator is used to separate water from the carbon dioxide, hydrogen, and alkane stream that is going to be fed in SEP-300.

To recover hydrogen from the aqueous phase reforming reactor, the vapor product is separated using pressure swing adsorption (PSA). Hydrogen, carbon dioxide, water, and various light alkanes are flowed across several adsorption columns at 20 bar. The 13x zeolite in the columns adsorb the polar components, alkanes, and carbon dioxide, while the hydrogen exits the column, unadsorbed. Once the column nears saturation, or the exit concentration of hydrogen falls below a desired point, the inlet and outlet valves are shut off and a small amount of product purity hydrogen is sent through the column, causing the polar components, alkanes, and carbon dioxide to desorb from the adsorbent and regenerate the column. Once the column is regenerated, the cycle is repeated. Multiple adsorption columns are necessary to make optimal use of the compressor and inlet streams, ensuring that at least one column is being fed gas at any point, preventing the need for a storage tank before the PSA.

Because pressure swing adsorption is a batch process, it was left out of the ASPEN simulation. On the block diagram for APR, it is represented by SEP-300. A storage tank is used to collect excess hydrogen from the adsorption columns so that downstream of the storage tank, the hydrogen appears to come from a continuous source.

Four columns are used for the PSA system in order to make the system as flexible as possible. Since some assumptions had to be made, it was decided to make a conservative estimate of the breakthrough time for each adsorber. Each adsorber will have gas flowed through it for 12
minutes, and then be desorbed at atmospheric pressure for 6 minutes. The adsorbers will start running at 0, 4, 8, and 12 minutes so that at any given moment three of the four adsorbers will be adsorbing gas, while one adsorber is being regenerated. This ensures the lowest flowrate possible through the adsorbers, which increases the amount of unwanted gases that adsorb to the zeolite, increasing the recovery of hydrogen. This schedule is summarized in Figure 3 (Cavenati, 2004).

**Figure 3**
Section III: Process Overview, Flowsheets, & Material Balances

Section 300: Aqueous Phase Reforming

Diagram of the process flow for Aqueous Phase Reforming.
<table>
<thead>
<tr>
<th></th>
<th>CW-300</th>
<th>CW-301</th>
<th>CW-304</th>
<th>S-225</th>
<th>S-300</th>
<th>S-301</th>
<th>S-302</th>
<th>S-303</th>
<th>S-304</th>
<th>S-305</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow (lb/hr)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>658083</td>
<td>131617</td>
<td>174447</td>
<td>174447</td>
<td>174447</td>
<td>174447</td>
<td>174447</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>13</td>
<td>13</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>89</td>
<td>89</td>
<td>89</td>
</tr>
<tr>
<td>Water</td>
<td>60786</td>
<td>60786</td>
<td>1395680</td>
<td>1395680</td>
<td>585695</td>
<td>117139</td>
<td>162433</td>
<td>162433</td>
<td>162433</td>
<td>162433</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydrosulfite</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowtherMA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr)| 3374   | 3374   | 77472  | 77472  | 36123  | 7225   | 9977   | 9977   | 9977   | 9977   |
| Total Flow (lb/hr)   | 60786  | 60786  | 1395680| 1395680| 1243780| 248756 | 336982 | 336982 | 336982 | 336982 |
| Total Flow (cuft/hr) | 987    | 1004   | 22057  | 23040  | 16938  | 3388   | 4751   | 4751   | 4825   | 5173   |
| Temperature (°F)     | 90.0   | 120.67 | 40.0   | 120.50 | 176.80 | 176.80 | 227.58 | 227.58 | 253.57 | 253.59 |
| Pressure (psia)      | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  | 14.70  |
| Vapor Fraction       | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |

Castillo, Ernst, Lerch, Winchester

APR Stream Report (1 of 4)
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>42830</td>
<td>42830</td>
<td>42830</td>
<td>42830</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>27996</td>
<td>27996</td>
<td>13</td>
<td>13</td>
<td>27983</td>
<td>27983</td>
<td>27983</td>
<td>27983</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>93122</td>
<td>93122</td>
<td>89</td>
<td>89</td>
<td>91033</td>
<td>91033</td>
<td>91033</td>
<td>91033</td>
<td>91033</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>165664</td>
<td>165664</td>
<td>45294</td>
<td>45294</td>
<td>120370</td>
<td>120370</td>
<td>120370</td>
<td>120370</td>
<td>24372</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7370</td>
<td>7370</td>
<td>1</td>
<td>1</td>
<td>7369</td>
<td>7369</td>
<td>7369</td>
<td>7369</td>
<td>0</td>
<td>7369</td>
<td>7369</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Flow (lbmol/hr)</td>
<td>15838</td>
<td>15838</td>
<td>2752</td>
<td>2752</td>
<td>13086</td>
<td>13086</td>
<td>13086</td>
<td>13086</td>
<td>4101</td>
<td>3656</td>
<td>3656</td>
</tr>
<tr>
<td>Total Flow (lb/hr)</td>
<td>336982</td>
<td>336982</td>
<td>88227</td>
<td>88227</td>
<td>248756</td>
<td>248756</td>
<td>248756</td>
<td>248756</td>
<td>145387</td>
<td>7369</td>
<td>7369</td>
</tr>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>101208</td>
<td>101208</td>
<td>253325</td>
<td>253325</td>
<td>1380</td>
<td>1380</td>
<td>382110</td>
<td>6320480</td>
<td>5800240</td>
<td>1450210</td>
<td>24831</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>359.60</td>
<td>314.62</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
<td>359.60</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
<td>725.19</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>0.53</td>
<td>0.57</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.81</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>---------------------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>526467</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>27983</td>
<td>0</td>
<td>27983</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>468556</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1228</td>
<td>1228</td>
<td>1228</td>
<td>1228</td>
<td>1231</td>
<td>1228</td>
<td>7369</td>
<td>0</td>
<td>7369</td>
<td>7369</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Flow (lbmol/hr)</td>
<td>609</td>
<td>609</td>
<td>609</td>
<td>609</td>
<td>610</td>
<td>609</td>
<td>7757</td>
<td>5329</td>
<td>3656</td>
<td>13086</td>
<td>28899</td>
</tr>
<tr>
<td>Total Flow (lb/hr)</td>
<td>1228</td>
<td>1228</td>
<td>1228</td>
<td>1228</td>
<td>1231</td>
<td>1228</td>
<td>152756</td>
<td>96000</td>
<td>7369</td>
<td>248756</td>
<td>995023</td>
</tr>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>3693</td>
<td>3693</td>
<td>3693</td>
<td>3693</td>
<td>3702</td>
<td>3693</td>
<td>3390850</td>
<td>1603</td>
<td>1601510</td>
<td>2720670</td>
<td>13550</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>175.73</td>
<td>140.00</td>
<td>140.00</td>
<td>140.00</td>
<td>140.00</td>
<td>176.80</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>1164.30</td>
<td>1164.30</td>
<td>1164.30</td>
<td>1164.30</td>
<td>1164.30</td>
<td>1164.30</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>17.70</td>
<td>741.70</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.57</td>
<td>0.00</td>
</tr>
</tbody>
</table>
### APR Stream Report (4 of 4)

<table>
<thead>
<tr>
<th></th>
<th>S-401</th>
<th>S-402</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass Flow (lb/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>526467</td>
<td>526467</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Water</strong></td>
<td>468556</td>
<td>468556</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Napthalene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Total Flow (lbmol/hr)</strong></td>
<td>28899</td>
<td>28899</td>
</tr>
<tr>
<td><strong>Total Flow (lb/hr)</strong></td>
<td>995023</td>
<td>995023</td>
</tr>
<tr>
<td><strong>Total Flow (cuft/hr)</strong></td>
<td>13552</td>
<td>13757</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>176.99</td>
<td>204.16</td>
</tr>
<tr>
<td><strong>Pressure (psia)</strong></td>
<td>667.70</td>
<td>667.70</td>
</tr>
<tr>
<td><strong>Vapor Fraction</strong></td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Section 400: Condensation

The condensation reaction converts sorbitol produced during hydrolysis and hydrogenation into water and a mixture of alkane and aromatic products that includes the final product, para-xylene. In the reactor, water and hydrogen vapor are driven off during the formation of the new carbon-carbon bonds present in the final product. In theory, any sugar alcohol or other “oxygenated hydrocarbon” can be used; in particular, US patent 2008/0300435 A1 contained one example with an acetone feed over gallium-loaded catalyst which converts nearly 80% of carbon in the feed into aromatics. However, the current design relies on a feed containing 50% sorbitol by mass in order to maintain comparability with other examples in the literature; consequently, the process only achieves a single pass yield of 48.4% aromatics. Other patents, such as US Patent 6372680, report less specific but similar results.

Catalyst

An activated zeolite or aluminosilicate catalyst, normally pentasil (more commonly called ZSM-5), facilitates the reaction. Zeolites have a porous structure that can accommodate a wide variety of cations. The cations are loosely held and exchange easily with cations in the contacted solution. Similar catalysts are used in the aqueous phase reforming and transalkylation portions of this process, and information on their manufacture and properties can be found in US patent 2008/0300435 A1. For the condensation of sorbitol to produce para-xylene, ZSM-5, with a thirty-to-one silicon dioxide to aluminum oxide ratio, is treated with a gallium nitrate solution, dried overnight in a vacuum oven, and subsequently calcined in flowing air at 400 degrees Celsius to effect 1.2% loading by weight of gallium (Example 46 in the patent). The prior cost-benefit analysis favors purchasing the catalyst from an external supplier to manufacturing the catalyst in-house.

Pre-Heating and Depressurization
Section III: Process Overview, Flowsheets, & Material Balances

The condensation section of the process begins with a valve, VAL-400), which releases the excess pressure generated during the aqueous phase reforming in order to establish conditions suitable for condensation. The outlet pressure is specified at 653 psig, which results in a 74 psig pressure drop across the valve.

Between the valve and reactor is a series of four heat exchangers (HX-400, HX-402, HX-403, HX-404), each followed by a small pump (P-400, P-401, P-402, P-403) that restores pressure lost to friction with a 2 psi pressure increase (industry heuristic). The heat exchangers then transfer heat from the hydrogen APR product, the pre-crystallization para-xylene stream, the transalkylation product, and the hot Dowtherm A stream to the condensation feed, respectively. Each exchanger conservatively assumes an overall heat transfer coefficient, U, of 50 BTU per hr-ft²-Rankine (Product and Process Design Principles; hereafter, PPDP) and allows for a conservative minimum temperature approach of 20 degrees Fahrenheit. The first exchanger (HX-400) is specified such that outlet temperatures approach to within 50 degrees Fahrenheit; this maximizes heat transfer while abiding by industry heuristics for streams above 300 degrees Fahrenheit. The second exchanger brings the pre-crystallization xylene stream and condensation feed to within 20 degrees Fahrenheit; this maximizes heat transfer while abiding by industry heuristics for streams under 300 degrees Fahrenheit. The third exchanger brings the transalkylation product and feed to within 50 degrees Fahrenheit; again, this maximizes heat transfer subject to heuristic-based constraints on the minimum allowable temperature approach. The fourth exchanger provides the final requisite heat to the condensation feed while cooling the refrigerant, Dowtherm A; this serves the simultaneous purpose of cooling the Dowtherm A in the refrigeration cycle used to cool the xylene stream for crystallization. See Figure 4 for a summary.
Figure 4

The feed is then split into four equal streams using a conventional splitter (Spt-401) and fed into four identical condensation reactors; a single reactor would be prohibitively large. Specifically, the splitter takes a 995,000 lb/hr aqueous feed of 50% sorbitol (by mass) at 698 degrees Fahrenheit and 642 psia and splits it into four 249,000 lb/hr streams of the same composition, temperature, and pressure. Each reactor (R-400, R-401, R-402, and R-403) is an identical packed bed reactor, operated at 625 psig and 370 degrees Celsius, as specified in example 55 (PP) of US patent 2008/0300435 A1, and catalyzed by the catalyst prescribed in example 46 of the same. Each processes a 249,000 lb/hr feed stream of 50% sorbitol (by mass) in water. In ASPEN, the reactors were modeled using identical RYIELD blocks. Based on the information in Table 13 (pg. 37) and Figure 17, which offered mass fractions in the organic stream for generalized product categories (e.g. C5+ olefins), the following mass fractions were assumed for each representative species identified in Figure 5 below. Although some error is expected when manually interpreting figures, these estimates yielded an overall mass fraction of unity with very little post-measurement manipulation. Yields for the RYIELD blocks were then calculated for a pure sorbitol stream, then adjusted to account for the 50% water by mass in the feed, as illustrated in Figure 5.
Section III: Process Overview, Flowsheets, & Material Balances

**Figure 5**

<table>
<thead>
<tr>
<th>Product</th>
<th>Molar mass</th>
<th>C</th>
<th>H</th>
<th>O</th>
<th>Mass fraction in organic</th>
<th>Mole fraction in organic</th>
<th>Yield from Sorbitol</th>
<th>ASPEN Yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>182.17</td>
<td>6</td>
<td>14</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>o-xylene</td>
<td>106.16</td>
<td>8</td>
<td>10</td>
<td>0</td>
<td>0.2037</td>
<td>0.1854</td>
<td>0.46606</td>
<td>0.04145</td>
</tr>
<tr>
<td>o-xylene</td>
<td>106.16</td>
<td>8</td>
<td>10</td>
<td>0</td>
<td>0.0038</td>
<td>0.0034</td>
<td>0.00865</td>
<td>0.00077</td>
</tr>
<tr>
<td>m-xylene</td>
<td>106.16</td>
<td>8</td>
<td>10</td>
<td>0</td>
<td>0.0004</td>
<td>0.0004</td>
<td>0.00056</td>
<td>0.00009</td>
</tr>
<tr>
<td>ethylbenzene</td>
<td>106.16</td>
<td>8</td>
<td>10</td>
<td>0</td>
<td>0.0023</td>
<td>0.0019</td>
<td>0.00480</td>
<td>0.00049</td>
</tr>
<tr>
<td>toluene</td>
<td>92.14</td>
<td>7</td>
<td>8</td>
<td>0</td>
<td>0.0450</td>
<td>0.0472</td>
<td>0.10380</td>
<td>0.00916</td>
</tr>
<tr>
<td>benzene</td>
<td>81.11</td>
<td>6</td>
<td>6</td>
<td>0</td>
<td>0.0100</td>
<td>0.0124</td>
<td>0.02332</td>
<td>0.00204</td>
</tr>
<tr>
<td>1,2,4-trimethylbenzene</td>
<td>120.19</td>
<td>9</td>
<td>12</td>
<td>0</td>
<td>0.1000</td>
<td>0.1206</td>
<td>0.34103</td>
<td>0.03093</td>
</tr>
<tr>
<td>isopropylbenzene</td>
<td>120.19</td>
<td>9</td>
<td>12</td>
<td>0</td>
<td>0.1500</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Naphthalene</td>
<td>128.17</td>
<td>10</td>
<td>8</td>
<td>0</td>
<td>0.2000</td>
<td>0.0754</td>
<td>0.29689</td>
<td>0.02033</td>
</tr>
<tr>
<td>butane</td>
<td>56.12</td>
<td>4</td>
<td>10</td>
<td>0</td>
<td>0.0300</td>
<td>0.0459</td>
<td>0.06269</td>
<td>0.00611</td>
</tr>
<tr>
<td>pentane</td>
<td>72.15</td>
<td>5</td>
<td>12</td>
<td>0</td>
<td>0.1150</td>
<td>0.1540</td>
<td>0.24157</td>
<td>0.02240</td>
</tr>
<tr>
<td>hexane</td>
<td>86.18</td>
<td>6</td>
<td>14</td>
<td>0</td>
<td>0.1600</td>
<td>0.1794</td>
<td>0.33821</td>
<td>0.03256</td>
</tr>
<tr>
<td>heptane</td>
<td>100.2</td>
<td>7</td>
<td>10</td>
<td>0</td>
<td>0.0350</td>
<td>0.0538</td>
<td>0.07424</td>
<td>0.00712</td>
</tr>
<tr>
<td>butene</td>
<td>56.1</td>
<td>4</td>
<td>8</td>
<td>0</td>
<td>0.0048</td>
<td>0.0083</td>
<td>0.01042</td>
<td>0.00098</td>
</tr>
<tr>
<td>pentene</td>
<td>70.13</td>
<td>5</td>
<td>10</td>
<td>0</td>
<td>0.0145</td>
<td>0.0200</td>
<td>0.03144</td>
<td>0.00290</td>
</tr>
<tr>
<td>hexene</td>
<td>84.16</td>
<td>6</td>
<td>12</td>
<td>0</td>
<td>0.0262</td>
<td>0.0232</td>
<td>0.04375</td>
<td>0.00411</td>
</tr>
<tr>
<td>heptene</td>
<td>98.18</td>
<td>7</td>
<td>14</td>
<td>0</td>
<td>0.0044</td>
<td>0.0044</td>
<td>0.00957</td>
<td>0.00090</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.9590</td>
<td>1.0000</td>
<td>20.35%</td>
<td>20.35%</td>
</tr>
</tbody>
</table>

*An oxygen balance shows that 59.3% of the yield from pure sorbitol is water, leaving 40.7% organic yield. With a 50% water feed, this leaves 20.35% total yield. To get ASPEN Yields, multiply organic mass fractions by this factor.*

**Post-Condensation Cooling and Heat Recovery**

After reacting, a mixer (MIX-400) takes each 249,000 lb/hr para-xylene-containing product stream at 698 degrees Fahrenheit and 640 psia, present entirely in the vapor phase, and combines them into a single 995,000 lb/hr stream at the same composition and conditions. A splitter (SPT-400) then splits this combined product stream into three 332,000 lb/hr streams for at the same composition and conditions; this provides three streams which can preheat the feed to each of the three Hydrolysis reactors.

Each of the three identical 332,000 lb/hr product streams, still hot, is then fed through one of three pre-hydrolysis heat exchangers (HX-100, HX-101, HX-102); these exchangers each cool an effluent stream while pre-heating a feed to one of three hydrolysis reactors. Each exchanger conservatively assumes an overall heat transfer coefficient, U, of 50 BTU per hr-ft²-Rankine (industry heuristic) and a minimum temperature approach of 20 degrees Fahrenheit. With these parameters, each exchanger then specified a cold stream outlet temperature of 212 degrees Fahrenheit, the desired temperature for hydrolysis. The partially-cooled reactor effluents exit each exchanger at 506 degrees Fahrenheit, well above the temperature desired for distillation. All three
Castillo, Ernst, Lerch, Winchester

streams are then combined by a mixer (MIX-401) for further phase and temperature changes prior to distillation.

The combined partially-cooled condensation product, flowing at 995,000 lb/hr, then passes through a valve (VAL-401) which vents the stream to a specified pressure of 1.5 psig. This pressure causes the condensation product to reach distillation at approximately atmospheric pressure. This pressure is cheap and easy to achieve; in addition, major components in the effluent can be isolated with high recoveries, and these distillations can all use cooling water to serve the condenser duties. The effluent then passes through a final heat exchanger (HX-401), which uses cooling water to cool the effluent to 50 degrees Celsius in anticipation of 3-phase separation. In accordance with industry standard, the heater specifies that cooling water that enters at 90 degrees Fahrenheit exit at 120. The flow rate of cooling water was then adjusted to 60,000 gallons per minute in order to achieve the desired hot-stream outlet temperature.
Section III: Process Overview, Flowsheets, & Material Balances

Section 400: Condensation
### Condensation Stream Report (1 of 3)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
<td>526467</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>468556</td>
<td>117139</td>
<td>117139</td>
<td>117139</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Dowtherm™</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

<p>| Total Flow (lb/hr) | 995023| 995023| 995023| 995023| 995023| 995023| 995023| 248756| 248756| 248756| 248756|
| Total Flow (cuft/hr)| 13550 | 13552 | 13757 | 13758 | 14561 | 14561 | 22455 | 22458 | 5614  | 5614  | 5614  |
| Temperature (°F)  | 176.80| 176.99| 204.16| 204.16| 298.62| 298.62| 698.10| 698.15| 698.15| 698.15| 698.15|
| Pressure (psia)   | 741.70| 667.70| 667.70| 669.70| 669.70| 671.70| 641.70| 641.70| 641.70| 641.70| 641.70|
| Vapor Fraction    | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| <strong>Mass Flow (lb/hr)</strong> | | | | | | | | | | |
| Sorbitol | 131617 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Para-Xylene | 0 | 10284 | 10284 | 10284 | 10284 | 41138 | 13712 | 13713 | 13712 | 13712 |
| Ortho-Xylene | 0 | 191 | 191 | 191 | 191 | 763 | 254 | 254 | 254 | 254 |
| Meta-Xylene | 0 | 21 | 21 | 21 | 21 | 85 | 28 | 28 | 28 | 28 |
| Methane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Ethane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Propane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| N-Butane | 0 | 1515 | 1515 | 1515 | 1515 | 6059 | 2020 | 2020 | 2020 | 2020 |
| N-Pentane | 0 | 5806 | 5806 | 5806 | 5806 | 23225 | 7741 | 7741 | 7741 | 7741 |
| N-Hexane | 0 | 8078 | 8078 | 8078 | 8078 | 32312 | 10771 | 10771 | 10771 | 10771 |
| Carbon Dioxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Water | 117139 | 198222 | 198222 | 198222 | 198222 | 792890 | 264294 | 264302 | 264294 | 264294 |
| Hydrogen | 0 | 97 | 97 | 97 | 97 | 389 | 130 | 130 | 130 | 130 |
| Glucose | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Oxygen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Nitrogen | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Carbon Monoxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sucrose | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sodium Hydroxide | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Ethylbenzene | 0 | 106 | 106 | 106 | 106 | 424 | 141 | 141 | 141 | 141 |
| Toluene | 0 | 2272 | 2272 | 2272 | 2272 | 9087 | 3029 | 3029 | 3029 | 3029 |
| Benzene | 0 | 505 | 505 | 505 | 505 | 2019 | 673 | 673 | 673 | 673 |
| Naphthalene | 0 | 5049 | 5049 | 5049 | 5049 | 20195 | 6732 | 6732 | 6732 | 6732 |
| 1,2,4-Trimethylbenzene | 0 | 5049 | 5049 | 5049 | 5049 | 20195 | 6732 | 6732 | 6732 | 6732 |
| Isopropylbenzene | 0 | 7575 | 7575 | 7575 | 7575 | 30293 | 10098 | 10098 | 10098 | 10098 |
| N-Heptane | 0 | 1767 | 1767 | 1767 | 1767 | 7068 | 2356 | 2356 | 2356 | 2356 |
| 1-Butene | 0 | 243 | 243 | 243 | 243 | 972 | 324 | 324 | 324 | 324 |
| 1-Pentene | 0 | 733 | 733 | 733 | 733 | 2934 | 978 | 978 | 978 | 978 |
| 1-Hexene | 0 | 223 | 223 | 223 | 223 | 893 | 298 | 298 | 298 | 298 |
| Air | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| DowthermA | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| <strong>Total Flow (lbmol/hr)</strong> | 7225 | 11574 | 11574 | 11574 | 11574 | 46295 | 15432 | 15432 | 15432 | 15432 |
| <strong>Total Flow (lb/hr)</strong> | 248756 | 248756 | 248756 | 248756 | 248756 | 995023 | 331671 | 331681 | 331671 | 331671 |
| <strong>Total Flow (cuft/hr)</strong> | 5614 | 205500 | 205500 | 205500 | 205500 | 823002 | 273998 | 274006 | 273998 | 208888 |
| <strong>Temperature (°F)</strong> | 698.15 | 698.00 | 698.00 | 698.00 | 698.00 | 698.00 | 698.00 | 698.00 | 505.98 | 505.98 |
| <strong>Pressure (psia)</strong> | 641.70 | 639.70 | 639.70 | 639.70 | 639.70 | 639.70 | 639.70 | 639.70 | 639.70 | 639.70 |
| <strong>Vapor Fraction</strong> | 0.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |</p>
<table>
<thead>
<tr>
<th>Compounds</th>
<th>S-422</th>
<th>S-425</th>
<th>S-426</th>
<th>S-507</th>
<th>S-520</th>
<th>S-601</th>
<th>S-602</th>
<th>S-603</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>526467</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>13713</td>
<td>41138</td>
<td>0</td>
<td>53820</td>
<td>53820</td>
<td>18807</td>
<td>18807</td>
<td>18807</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>254</td>
<td>763</td>
<td>0</td>
<td>3249</td>
<td>3249</td>
<td>2739</td>
<td>2739</td>
<td>2739</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>28</td>
<td>85</td>
<td>0</td>
<td>5089</td>
<td>5089</td>
<td>5478</td>
<td>5478</td>
<td>5478</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>2020</td>
<td>6059</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>7742</td>
<td>23225</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>10771</td>
<td>32312</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>264302</td>
<td>792890</td>
<td>468556</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>130</td>
<td>389</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>141</td>
<td>424</td>
<td>0</td>
<td>835</td>
<td>835</td>
<td>548</td>
<td>548</td>
<td>548</td>
</tr>
<tr>
<td>Toluene</td>
<td>3029</td>
<td>9087</td>
<td>0</td>
<td>2374</td>
<td>2374</td>
<td>135120</td>
<td>135120</td>
<td>135120</td>
</tr>
<tr>
<td>Benzene</td>
<td>673</td>
<td>2019</td>
<td>0</td>
<td>0</td>
<td>19903</td>
<td>19903</td>
<td>19903</td>
<td>19903</td>
</tr>
<tr>
<td>Napthalene</td>
<td>6732</td>
<td>20195</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>6732</td>
<td>20195</td>
<td>0</td>
<td>133</td>
<td>133</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>10098</td>
<td>30293</td>
<td>0</td>
<td>13174</td>
<td>13174</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>2356</td>
<td>7068</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>324</td>
<td>972</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>384</td>
<td>384</td>
<td>384</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>978</td>
<td>2934</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>1361</td>
<td>4081</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>298</td>
<td>893</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Total Flow (lb/hr)</strong></td>
<td>331681</td>
<td>995023</td>
<td>995023</td>
<td>78674</td>
<td>78674</td>
<td>203468</td>
<td>203468</td>
<td>203468</td>
</tr>
<tr>
<td><strong>Total Flow (lbmol/hr)</strong></td>
<td>15432</td>
<td>46295</td>
<td>28899</td>
<td>730</td>
<td>730</td>
<td>2281</td>
<td>2281</td>
<td>2281</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>505.98</td>
<td>122.00</td>
<td>206.67</td>
<td>282.70</td>
<td>226.67</td>
<td>850.00</td>
<td>348.63</td>
<td>182.00</td>
</tr>
<tr>
<td>Pressure (psia)</td>
<td>639.70</td>
<td>16.20</td>
<td>669.70</td>
<td>14.70</td>
<td>14.70</td>
<td>164.70</td>
<td>164.70</td>
<td>164.70</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>1.00</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Condensation Stream Report (3 of 3)
Section 500: Separations

Distillation Columns

The separation scheme has four columns, DC-500, DC-501, DC-502, and DC-503. DC-500 and DC-501 follow the condensation, while DC-502 and DC-503 follow the transalkylation. DC-500 is a 30-tray separation between toluene and para-xylene. It’s fed with a combination of effluent from the condensation reactor and a recycled stream of additional para-xylene and leftover toluene from DC-502 in the post-transalkylation separation. The distillate feeds the transalkylation reactor, while the bottoms product is sent to DC-501 for further separation. DC-501 then separates the xylene isomers, now the lightest components, from the other heavy components. The xylenes are sent for crystallization to isolate the para-isomer, and the heavy components are sent to the furnace to offset utilities. DC-502 follows the transalkylation, and separates benzene and lighter components from the heavier toluene and xylenes to be sent back DC-500. The distillate from DC-502 is then fed to DC-503, which separates lighter hydrocarbon side products, which can be burned to offset utilities, from valuable benzene, which can be sold for additional revenue. This scheme separates valuable components using the lowest possible number of distillation columns.

Columns were designed by modifying a McCabe-Thiele analysis. The McCabe-Thiele diagrams in Appendix B were generated by ignoring the presence of species that were neither the light nor heavy key. The columns were initially modeled after these diagrams. If ASPEN indicated a tendency for trays to dry out, the reflux ratio was increased in increments of 1 until the simulation successfully converged. Then, the distillate to feed ratio was adjusted to maximize light key recovery and minimize heavy key recovery. After achieving the desired separation, the idealized profile was translated into a more realistic set of trays and non-unity efficiencies using the O’Connell correlation. These calculations can be found in Appendix B. In all cases, these “real” columns performed separations that were nearly identical to their ideal counterparts.
Section 500: Distillation Subsection 1
Section III: Process Overview, Flowsheets, & Material Balances

Section 500: Distillation Subsection 2
Crystallization

Crystallization is often used when para-xylene is mixed with other xylenes and ethylbenzene, but it can also be used for our scenario where there is a significant proportion of isopropylbenzene and toluene. As the freezing point of isopropylbenzene and toluene are considerably lower than meta-xylene and ortho-xylene (see Figure 6), it can be assumed that crystallization will work just as well, if not better at -30 °C, for a system including isopropylbenzene and toluene.

The xylenes product from the distillation columns is fed to a scraped surface crystallizer (SSC) with a cooling jacket. The SSC cools the solution of para-xylene, meta-xylene, ortho-xylene, isopropylbenzene, toluene, ethylbenzene and other aromatics to -30 °C which causes pure para-xylene crystals to form on the surface of the crystallizer. The scrapers, which rotate at 12 rpm, free the crystals and allow them to be fed into a washing column as a suspension in the mother liquor. The washing column consists of a piston with a filter attached to its face and a scraper at the bottom of the column. Washing takes place in four steps. In the first step, the piston is lifted to allow the crystal suspension to fill the column. The inlet is then shut off and an outlet above the piston is opened and the piston is forced downward, causing the mother liquor to flow through the filter on the piston. In the third step product purity para-xylene is fed through the bottom of the column, washing the crystals. For the final step the scraper is rotated as the piston continues to push downwards, grinding the crystals into smaller fragments that are carried through the bottom of the column and melt into the para-xylene product.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Normal Boiling Point (°C)</th>
<th>Freezing Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Para-Xylene</td>
<td>138</td>
<td>13</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>139</td>
<td>-48</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>144</td>
<td>-25.2</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>136</td>
<td>-95</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>152</td>
<td>-96</td>
</tr>
<tr>
<td>Toluene</td>
<td>111</td>
<td>-95</td>
</tr>
</tbody>
</table>
Section 500: Crystallization Subsection

Aromatics To Furnace

Perxylene Product

Crystallizer

Xylenes From Separation

Sorbitol To Condensation

HK-01

HK-02

S-403

S-426

S-507

S-520

S-521

HK-301

CRY-500

S-009

S-510

72
### Section III: Process Overview, Flowsheets, & Material Balances

#### Separation Stream Report (1 of 2)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow (lb/hr)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0 0 14138</td>
<td>41138</td>
<td>41138</td>
<td>492</td>
<td>40646</td>
<td>0</td>
<td>40646</td>
<td>59451</td>
<td>53936</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0 0 763</td>
<td>763</td>
<td>763</td>
<td>8</td>
<td>756</td>
<td>0</td>
<td>756</td>
<td>3495</td>
<td>3365</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0 0 85</td>
<td>85</td>
<td>85</td>
<td>1</td>
<td>84</td>
<td>0</td>
<td>84</td>
<td>5561</td>
<td>5103</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Methane</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0 0 6059</td>
<td>6059</td>
<td>6059</td>
<td>3464</td>
<td>2595</td>
<td>0</td>
<td>2595</td>
<td>2595</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0 0 23225</td>
<td>23225</td>
<td>23225</td>
<td>7254</td>
<td>15971</td>
<td>0</td>
<td>15971</td>
<td>15976</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0 0 32312</td>
<td>32312</td>
<td>32312</td>
<td>4472</td>
<td>27840</td>
<td>0</td>
<td>27840</td>
<td>27840</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>29651800</td>
<td>29651800</td>
<td>792890</td>
<td>792890</td>
<td>792890</td>
<td>978</td>
<td>1697</td>
<td>790215</td>
<td>1697</td>
<td>1697</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0 0 389</td>
<td>389</td>
<td>389</td>
<td>388</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Glucose</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0 0 424</td>
<td>424</td>
<td>424</td>
<td>6</td>
<td>418</td>
<td>0</td>
<td>418</td>
<td>966</td>
<td>836</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Toluene</td>
<td>0 0 9087</td>
<td>9087</td>
<td>9087</td>
<td>295</td>
<td>8792</td>
<td>0</td>
<td>8792</td>
<td>135420</td>
<td>2374</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>0 0 2019</td>
<td>2019</td>
<td>2019</td>
<td>200</td>
<td>1819</td>
<td>0</td>
<td>1819</td>
<td>2479</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0 0 20195</td>
<td>20195</td>
<td>20195</td>
<td>16</td>
<td>20179</td>
<td>0</td>
<td>20179</td>
<td>20179</td>
<td>20179</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0 0 20195</td>
<td>20195</td>
<td>20195</td>
<td>69</td>
<td>20126</td>
<td>0</td>
<td>20126</td>
<td>20126</td>
<td>20113</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0 0 30293</td>
<td>30293</td>
<td>30293</td>
<td>222</td>
<td>30071</td>
<td>0</td>
<td>30071</td>
<td>30071</td>
<td>29739</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0 0 7068</td>
<td>7068</td>
<td>7068</td>
<td>391</td>
<td>6677</td>
<td>0</td>
<td>6677</td>
<td>6677</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Butene</td>
<td>0 0 972</td>
<td>972</td>
<td>972</td>
<td>589</td>
<td>384</td>
<td>0</td>
<td>384</td>
<td>384</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0 0 2934</td>
<td>2934</td>
<td>2934</td>
<td>1016</td>
<td>1918</td>
<td>0</td>
<td>1918</td>
<td>1919</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0 0 4081</td>
<td>4081</td>
<td>4081</td>
<td>642</td>
<td>3440</td>
<td>0</td>
<td>3440</td>
<td>3440</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>0 0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DowthermA</td>
<td>0 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Total Flow (lbmol/hr)

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Flow (lbmol/hr)</td>
<td>1645920</td>
<td>1645920</td>
<td>46295</td>
<td>46295</td>
<td>46295</td>
<td>509</td>
<td>1922</td>
<td>43864</td>
<td>1922</td>
<td>3565</td>
<td>1194</td>
</tr>
</tbody>
</table>

### Total Flow (lb/hr)

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Flow (cuft/hr)</td>
<td>481250</td>
<td>489452</td>
<td>626674</td>
<td>26662000</td>
<td>937806</td>
<td>213811</td>
<td>3797</td>
<td>13056</td>
<td>3797</td>
<td>6988</td>
<td>2814</td>
</tr>
</tbody>
</table>

### Temperature (°F)

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°F)</td>
<td>90.00</td>
<td>120.33</td>
<td>505.98</td>
<td>413.88</td>
<td>122.00</td>
<td>122.00</td>
<td>122.00</td>
<td>122.00</td>
<td>122.00</td>
<td>122.01</td>
<td>174.18</td>
</tr>
</tbody>
</table>

### Pressure (psia)

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
</table>

### Vapor Fraction

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor Fraction</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.05</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
### Separation Stream Report (2 of 2)

<table>
<thead>
<tr>
<th>Mass Flow (lb/hr)</th>
<th>S-506</th>
<th>S-507</th>
<th>S-508</th>
<th>S-510</th>
<th>S-511</th>
<th>S-512</th>
<th>S-514</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>53936</td>
<td>53820</td>
<td>53820</td>
<td>50322</td>
<td>116</td>
<td>5515</td>
<td>18805</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>3365</td>
<td>3249</td>
<td>3249</td>
<td>0</td>
<td>115</td>
<td>130</td>
<td>2739</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>5103</td>
<td>5089</td>
<td>5089</td>
<td>0</td>
<td>15</td>
<td>458</td>
<td>5477</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2595</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>15976</td>
<td>5</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>27840</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1697</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>836</td>
<td>835</td>
<td>835</td>
<td>0</td>
<td>1</td>
<td>130</td>
<td>548</td>
</tr>
<tr>
<td>Toluene</td>
<td>2374</td>
<td>2374</td>
<td>2374</td>
<td>0</td>
<td>0</td>
<td>133046</td>
<td>126627</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2479</td>
<td>659</td>
</tr>
<tr>
<td>Napthalene</td>
<td>20179</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>20179</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20113</td>
<td>133</td>
<td>133</td>
<td>0</td>
<td>19981</td>
<td>13</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>29739</td>
<td>13174</td>
<td>13174</td>
<td>0</td>
<td>16564</td>
<td>332</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6677</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>384</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1919</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3440</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>838</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Dowtherma</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr) | 1194 | 730 | 730 | 474 | 464 | 2371 | 1642 |
| Total Flow (lb/hr)    | 135645 | 78674 | 78674 | 50322 | 56971 | 203468 | 154861 |
| Total Flow (cuft/hr)  | 2814 | 1669 | 1389 | 888 | 1157 | 1117480 | 3196 |
| Temperature (°F)      | 300.54 | 282.70 | -22.00 | -22.00 | 341.89 | 207.92 | 239.18 |
| Pressure (psia)       | 16.70 | 14.70 | 14.70 | 14.70 | 14.70 | 14.70 | 16.70 |
| Vapor Fraction        | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 | 0.00 |
## Distillation Stream Report (1 of 1)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow (lb/hr)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>18805</td>
<td>18805</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>18807</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>2739</td>
<td>2739</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2739</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>5447</td>
<td>5447</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>5478</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
<td>2590</td>
<td>5</td>
<td>2595</td>
<td></td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>5</td>
<td>5</td>
<td>15971</td>
<td>15971</td>
<td>15971</td>
<td>15041</td>
<td>930</td>
<td>15976</td>
<td></td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>659777</td>
<td>659777</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>548</td>
<td>548</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>548</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>126627</td>
<td>126627</td>
<td>8493</td>
<td>8493</td>
<td>8493</td>
<td>0</td>
<td>8493</td>
<td>135120</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>659</td>
<td>659</td>
<td>19244</td>
<td>19244</td>
<td>19244</td>
<td>119</td>
<td>19125</td>
<td>19903</td>
</tr>
<tr>
<td>Napthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>1</td>
<td>384</td>
<td></td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1918</td>
<td>1918</td>
<td>1918</td>
<td>1828</td>
<td>90</td>
<td>1919</td>
<td></td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Total Flow (lbmol/hr)</strong></td>
<td>36623</td>
<td>36623</td>
<td>1642</td>
<td>1642</td>
<td>639</td>
<td>639</td>
<td>639</td>
<td>287</td>
<td>351</td>
<td>2281</td>
</tr>
<tr>
<td><strong>Total Flow (lb/hr)</strong></td>
<td>659777</td>
<td>659777</td>
<td>154861</td>
<td>154861</td>
<td>48607</td>
<td>48607</td>
<td>48607</td>
<td>19960</td>
<td>28646</td>
<td>203468</td>
</tr>
<tr>
<td><strong>Total Flow (cuft/hr)</strong></td>
<td>10427</td>
<td>10499</td>
<td>3196</td>
<td>3196</td>
<td>270204</td>
<td>1036</td>
<td>1036</td>
<td>110213</td>
<td>573</td>
<td>4203</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>40.0</td>
<td>53.18</td>
<td>239.17</td>
<td>239.18</td>
<td>139.86</td>
<td>62.80</td>
<td>62.82</td>
<td>86.09</td>
<td>175.69</td>
<td>182.01</td>
</tr>
<tr>
<td><strong>Pressure (psia)</strong></td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>14.70</td>
<td>16.70</td>
<td>14.70</td>
<td>16.70</td>
<td>166.70</td>
</tr>
<tr>
<td><strong>Vapor Fraction</strong></td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
## Crystallization Stream Report (1 of 1)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>526467</td>
<td>526467</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>53820</td>
<td>53820</td>
<td>3498</td>
<td>50322</td>
<td>53820</td>
<td>53820</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>3249</td>
<td>3249</td>
<td>3249</td>
<td>0</td>
<td>3249</td>
<td>3249</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>5089</td>
<td>5089</td>
<td>5089</td>
<td>0</td>
<td>5089</td>
<td>5089</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>468556</td>
<td>468556</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>835</td>
<td>835</td>
<td>835</td>
<td>0</td>
<td>835</td>
<td>835</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>2374</td>
<td>2374</td>
<td>2374</td>
<td>0</td>
<td>2374</td>
<td>2374</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Napthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>133</td>
<td>133</td>
<td>133</td>
<td>0</td>
<td>133</td>
<td>133</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>13174</td>
<td>13174</td>
<td>13174</td>
<td>0</td>
<td>13174</td>
<td>13174</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr) | 28899 | 28899 | 730   | 730   | 256   | 474   | 730   | 730   |
| Total Flow (lb/hr)    | 995023| 995023| 78674 | 78674 | 28352 | 50322 | 78674 | 78674 |
| Total Flow (cuft/hr)  | 13758 | 13777 | 1669  | 1389  | 501   | 888   | 1603  | 1449  |
| Temperature (°F)      | 204.16| 206.67| 282.70| -22.00| -22.00| -22.00| 60.00 | 60.00 |
| Pressure (psia)       | 669.70| 669.70| 14.70 | 14.70 | 14.70 | 14.70 | 14.70 | 14.70 |
| Vapor Fraction        | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  | 0.00  |
Section 600: Transalkylation

In transalkylation, side-products from the condensation reaction are converted into additional para-xylene. Because information on the possible products of condensation was limited, a large fraction of sorbitol was converted into undesired side-products. Transalkylation emerged as a way to recover some of this material, which would otherwise be burned or wasted. In addition, transalkylation simultaneously produced additional benzene, increasing benzene production to quantities significant enough to isolate and sell for additional revenue.

Of the available literature, US Patents 2011/0092756, 2005/0215839, and 6323381 provided the most complete and relevant information to the process at hand. This process’s transalkylation was modeled after Example 2 on column 10 of US Patent 6323381 due the specific yields presented and because of the selective production of para-xylene over its isomers, which was necessary to maintain a high enough concentration of the para-xylene isomer for crystallization.

Toluene-rich distillate from the first post-condensation separation, with toluene as the light key and para-xylene as the heavy key, feeds the transalkylation. The products are then separated into hydrocarbons for burning, benzene for separate sale, and heavier products for recycle and recovery.

Pre-Heating

Before transalkylation, the 200,000 lb/hr feed is vaporized in HX-600 and brought to the appropriate temperature of 850 degrees Fahrenheit. These conditions are specified by US patent 6323381. The heat duty of 68 million BTU/hr is provided by the furnace R-700. The stream is then fed to the transalkylation reactor R-600.

Transalkylation

The heated feed is fed continuously as one stream to a packed bed reactor at 850 degrees Fahrenheit and atmospheric pressure, as specified in US Patent 6323381. The yields were estimated
Castillo, Ernst, Lerch, Winchester  
from data provided in Example 2 of the aforementioned patent, with yields scaled to compensate for  
the absence of species such as heavy aromatics and xylene isomers in the feed.  

Transalkylation is catalyzed by zeolite catalyst, similar to the catalyzed condensation. In  
Example 2 of the aforementioned patent, a “selectivated large crystal HZSM-5 was used.” Although no further specifics were given, the catalyst was assumed similar enough to the condensation catalyst that both could be ordered together in order to achieve economies of scale. Information and assumptions applied to pricing for the condensation catalyst were also applied to the transalkylation catalyst.  

**Cooling and Heat Recovery**  
After exiting the reactor, the effluent pass through heat exchanger HX-403, where it  
simultaneously preheats feed for the condensation reaction. Nearly 80 million BTU/hr are transferred between streams. The exchanger is configured to maximize heat transfer by achieving the minimum allowable temperature approach of 50 degrees Fahrenheit for streams over 300 degrees Fahrenheit. The effluent then flows through heat exchanger HX-601, where cooling water is used to bring the stream to 128 degrees Fahrenheit; the flow rate of cooling water was adjusted such that the water enters at 90 degrees Fahrenheit and exits at 120, consistent with industry heuristics. Finally, pump P-601 provides a 2 psi increase to combat frictional pressure losses. The cooled effluent is then returned to the separation section of the process at distillation column DC-502.
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>526467</td>
<td>526467</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Para-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>5515</td>
<td>5515</td>
<td>18807</td>
<td>18807</td>
<td>18807</td>
<td>18807</td>
<td>18807</td>
</tr>
<tr>
<td>Ortho-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>130</td>
<td>130</td>
<td>2739</td>
<td>2739</td>
<td>2739</td>
<td>2739</td>
<td>2739</td>
</tr>
<tr>
<td>Meta-Xylene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>458</td>
<td>458</td>
<td>5478</td>
<td>5478</td>
<td>5478</td>
<td>5478</td>
<td>5478</td>
</tr>
<tr>
<td>Methane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Butane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
<td>2595</td>
</tr>
<tr>
<td>N-Pentane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
<td>15976</td>
</tr>
<tr>
<td>N-Hexane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>27840</td>
<td>27840</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>520883</td>
<td>520883</td>
<td>468556</td>
<td>468556</td>
<td>1697</td>
<td>1697</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Monoxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Sodium Hydroxide</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>130</td>
<td>130</td>
<td>548</td>
<td>548</td>
<td>548</td>
<td>548</td>
<td>548</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>133046</td>
<td>133046</td>
<td>135120</td>
<td>135120</td>
<td>135120</td>
<td>135120</td>
<td>135120</td>
</tr>
<tr>
<td>Benene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2479</td>
<td>2479</td>
<td>19903</td>
<td>19903</td>
<td>19903</td>
<td>19903</td>
<td>19903</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>13</td>
<td>13</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>332</td>
<td>332</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>6677</td>
<td>6677</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>384</td>
<td>384</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
<td>1919</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3440</td>
<td>3440</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>838</td>
<td>838</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Air</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DowthermA</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

| Total Flow (lbmol/hr) | 28913 | 28913 | 28899 | 28899 | 2371 | 2371 | 2281 | 2281 | 2281 | 2281 |
| Total Flow (lb/hr)    | 520883| 520883| 995023| 995023| 203468| 203468| 203468| 203468| 203468| 203468|
| Total Flow (cuft/hr)  | 8454  | 8599  | 14561 | 13777 | 1117480| 2258520| 185115| 4867  | 4203 | 4203 |
| Temperature (°F)      | 90.00 | 120.61| 298.62| 206.67| 800.00| 348.63| 180.00| 182.01| 182.01| 182.01|
| Pressure (psia)       | 14.70 | 14.70 | 669.70| 669.70| 14.70 | 14.70 | 164.70| 164.70| 164.70| 164.70|
| Vapor Fraction        | 0.00  | 0.00  | 0.00  | 1.00  | 1.00  | 1.00  | 0.00  | 0.00  | 0.00  | 0.00  |
Section 700: Furnace & Heating Cycles

The process requires a great deal of heating due to the extreme conditions of several reactors and to the utility-intensive distillation columns. Fortunately, a large number of alkanes and other combustible hydrocarbons are made available for combustion by Section 300 (aqueous phase reforming) and by Section 500 (separations). In order to minimize utilities, these by-products are combusted for one of three purposes: boiling steam, vaporizing Dowtherm A, or heating Solar Salt. A quick sanity check (see SC-700) shows that the process provides well over 977 MBtu/h for production of steam, which exceeds the total heating and steam requirements of 912 MBtu/h (see Figure 24).

**Molten Salt Furnace & Cycle**

The transalkylation reaction in reactor R-600 occurs at 850°F. Naturally, this requires extensive pre-heating of the feed (S-600) to the reactor. The most economical and environmentally-friendly material available at these temperatures is Solar Salt, a 60/40 mixture of sodium nitrate and potassium nitrate (other media considered are detailed in Table 18.1 of PPDP and in Mathur). Please see Section VIII and Appendix D for pricing and further materials specifications. After exiting a cone-roof storage tank (ST-701), the Solar Salt is heated in FRN-700 and travels through heat exchanger (HX-600), cooling from 1100°F to 900°F. The sensible heat transfer increases the temperature of the S-512 to 850°F.

**Dowtherm A Furnace & Cycle**

Acid-catalyzed condensation (R-400 through R-403) occurs in this process at 698°F - a temperature outside the reasonable reach of steam. Dowtherm A (product information in Appendix D) is sold by Dow Chemical Company, and is recommended for heating up to 750°F (Table 18.1, PPDP). The Dowtherm A is stored in a spherical tank, ST-700. Due to the large amount required, the stream splits into two, each of which travels through a separate furnace (FRN-701 and FRN-702).
before recombining as vapor and entering heat exchanger HX-404. The condensation of Dowtherm A provides the necessary heat to raise S-405 to the requisite 698°F.

**Fired Steam Boiler**

The four distillation column reboilers (RB-500 through RB-503), the crystallizer apparatus (CRY-500 and WC-500), and heat exchanger HX-301 require steam heating. Rather than purchase it externally, the heat is supplied by vaporizing excess water (S-526) in a fired steam boiler (FRN-703). The steam output is split as necessary according to Figure 7, with valves employed to adjust each stream to the required pressure.

### Figure 7

<table>
<thead>
<tr>
<th>Unit</th>
<th>Duty (Btu/h)</th>
<th>Temp (F)</th>
<th>Cond Temp (F)</th>
<th>Steam Pres (psig)</th>
<th>Utility Alternative (psig)</th>
<th>ΔH&lt;sub&gt;vap&lt;/sub&gt; (Btu/lb)</th>
<th>Amount (lb/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RB-500</td>
<td>75,402,272</td>
<td>296</td>
<td>341</td>
<td>126</td>
<td>150</td>
<td>875</td>
<td>86,174</td>
</tr>
<tr>
<td>RB-501</td>
<td>44,513,177</td>
<td>332</td>
<td>377</td>
<td>213</td>
<td>450</td>
<td>839</td>
<td>53,087</td>
</tr>
<tr>
<td>RB-502</td>
<td>146,774,702</td>
<td>239</td>
<td>284</td>
<td>52</td>
<td>50</td>
<td>922</td>
<td>159,192</td>
</tr>
<tr>
<td>RB-503</td>
<td>16,543,353</td>
<td>176</td>
<td>221</td>
<td>17</td>
<td>50</td>
<td>965</td>
<td>17,143</td>
</tr>
<tr>
<td>HX-301</td>
<td>32,323,000</td>
<td>360</td>
<td>405</td>
<td>260</td>
<td>450</td>
<td>822</td>
<td>39,327</td>
</tr>
<tr>
<td>WC-500</td>
<td>16,543,353</td>
<td>176</td>
<td>221</td>
<td>17</td>
<td>50</td>
<td>965</td>
<td>17,143</td>
</tr>
</tbody>
</table>
Section IV
Energy Balance
IV. ENERGY BALANCE & UTILITY REQUIREMENTS

An important specification of the project charter is to minimize utility usage and to ensure the project is “green.” This entails recycling as much water as possible, avoiding natural gases, and generally minimizing the carbon footprint. Regardless, the varied and at-times extreme conditions of the process require a variety of utilities for heating, cooling, and power. This section summarizes utility usage by type, describes assumptions and calculations, details cost-saving measures and their impact, and notes areas for further study.

Utility Requirements

Without integration or cost-saving measures, the process required electricity; steam at 50 psig, 150 psig, and 450 psig; cooling water; chilled water; refrigeration to -90°F; Dowtherm A; and molten salts. Due to the excess heat generated by burning by-products, all of the process steam requirements were quickly substituted with boiler feed water. In the final process design, however, excess water from the three-phase separation in Section 500 is used in place of externally-purchased boiler feed water, as well as to offset some cooling water requirements. This resulted in overall utility requirements as summarized in Figure 8.

Figure 8

<table>
<thead>
<tr>
<th>Utility</th>
<th>Annual Requirement</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity</td>
<td>159.33</td>
<td>GW</td>
</tr>
<tr>
<td>Cooling Water, 90°F</td>
<td>11.03</td>
<td>TBTU</td>
</tr>
<tr>
<td>Chilled Water, 40°F</td>
<td>5.73</td>
<td>GBTU</td>
</tr>
<tr>
<td>Refrigeration, -90°F</td>
<td>1.95</td>
<td>GBTU</td>
</tr>
<tr>
<td>Dowtherm A</td>
<td>4.20</td>
<td>GBTU</td>
</tr>
<tr>
<td>Molten Salt</td>
<td>491.04</td>
<td>MBTU</td>
</tr>
</tbody>
</table>

Amount and cost of utility are explored comparatively in Figure 9 and Figure 10.
The utilities are examined by type in the following sections, but more detailed information on cost is available in the Process Economics segment Utility Requirements.

**Electricity**

Electricity is needed for pumps throughout the process, as well as for a compressor and a washer-column unit. These latter two units are by far the largest consumers of electricity on a per-unit basis, with 83% and 5% of the overall consumption, respectively. See Figure 11.
Cooling Water

Cooling water is procured at 90°F for use in process heat exchangers, as well as distillation column condensers and in the multistage compressor’s intercoolers. See the summary in Figure 12. In all cases, the full temperature range of heating (up to 120°F) is used in order to minimize requirements while not violating Heuristic 27 (PPDP), which should prevent the worst of fouling. Note that one heat exchanger in particular, HX-401, is responsible for over 70% of the process cooling requirements. This unit should be further examined, as it represents a significant cost driver.
The total amount of cooling water used by this process, excluding HX-401 is 22,250 gpm, or about 10.5 billion gallons per year. Including HX-401, this increases dramatically to 82,250 gpm and 39.1 billion gallons per year.

**Chilled Water**

Chilled water is necessary to cool process streams to a minimum of 60°F. It is used in HX-500 to pre-cool the DC-503 inlet stream to the requisite 62.8°F (see Section 500). It is also used to minimize the amount of refrigeration required in block CRY-500, pre-cooling stream S-513. A total of 1,564 ton-day of chilled water is used. This equates to 2,650 gpm or 1.25 billion gallons per year.

**Refrigeration**

Refrigeration at -90°F is used in CRY-500 to crystallize para-xylene at -22°F. According to Table 18.1 of PPDP, vaporizing ethylene would be a more than adequate heat-transfer medium at this temperature range. The fluid is included in the overall purchase cost, according to the supplier.

**Dowtherm A**

Dowtherm A is a commonly employed heat source for temperatures outside the reasonable reach of steam, but not exceeding 750°F. In order to meet the process heating requirements in this
Section IV: Energy Balance & Utility Requirements

temperature range, about 532,000 pounds of Dowtherm A are required. Calculations are shown in SC-U00.

Molten Salt
Molten salts are employed to achieve temperatures up to 1,100°F. The transalkylation reaction in R-600 takes place at 850°F, and thus requires a medium like this. Solar Salt, detailed in Section -700 and in Appendix D is the molten salt used in this process. Given the residence time of six hours, around seven million pounds are necessary to achieve the required pre-heating of the feed. An example calculation is in SC-U00.

Cost-Saving Measures

Heat Integration
The process uses a multitude of heat exchangers in order to maximize energy efficiency. As a result, no externally-supplied steam or electric heating is required. See process overview and unit descriptions for more information.

Steam Generation
Excess process heat is used to vaporize water and produce steam for use in reboilers, HX-301, and SEP-500.

Excess Water Utilization
Both aqueous phase reforming (R-300) and condensation (R-40X) produce water, which is recovered after separations in streams S-324 and S-502, respectively. Both of these water supplies are extremely pure, but are at temperatures too high for use as cooling water. However, a portion of this water (S-527) is used in heat exchanger HX-601 to cool an inlet stream that exceeds 400°F (p.471, PPDP). The remaining excess water (S-324 and S-526) is used as boiler feed, which replaces the need for any external purchase. Note that the amount of excess water available for use as boiler feed exceeds that needed to meet steam requirements.
Impact of Cost-Saving Measures

In total, these cost-saving measures reduced utilities by $12.7 million per year. Figure 13 summarizes the savings, and calculations are shown in SC-U01.

Figure 13

<table>
<thead>
<tr>
<th>Initial Utility</th>
<th>Initial Amount</th>
<th>Unit</th>
<th>Initial Annual Utility Cost</th>
<th>Substitute Utility</th>
<th>Substitute Amount</th>
<th>Unit</th>
<th>Substitute Annual Utility Cost</th>
<th>Annual Savings</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam - 50 psig</td>
<td>193,478 lb/h</td>
<td>gpm</td>
<td>$4,597,047</td>
<td>Boiler Feed Water</td>
<td>388 gpm</td>
<td>$</td>
<td>311,518</td>
<td>$4,265,529</td>
</tr>
<tr>
<td>Steam - 150 psig</td>
<td>86,174 lb/h</td>
<td>gpm</td>
<td>$3,273,992</td>
<td>Boiler Feed Water</td>
<td>170 gpm</td>
<td>$</td>
<td>147,656</td>
<td>$3,128,336</td>
</tr>
<tr>
<td>Steam - 450 psig</td>
<td>92,414 lb/h</td>
<td>gpm</td>
<td>$4,850,656</td>
<td>Boiler Feed Water</td>
<td>185 gpm</td>
<td>$</td>
<td>158,348</td>
<td>$4,672,309</td>
</tr>
<tr>
<td>Boiler Feed Water</td>
<td>745 gpm</td>
<td></td>
<td>$637,521</td>
<td>Excess Water</td>
<td>745 gpm</td>
<td>$</td>
<td>-</td>
<td>$637,521</td>
</tr>
<tr>
<td>Cooling Water</td>
<td>1,003 gpm</td>
<td></td>
<td>$35,748</td>
<td>Excess Water</td>
<td>1,003 gpm</td>
<td>$</td>
<td>-</td>
<td>$35,748</td>
</tr>
</tbody>
</table>

Total Annual Savings: $12,739,442

Further Exploration

Excess Boiler Feed Water and Steam Turbines

Generation of electricity via steam turbines should be explored as a means of work-integration and cost saving. Streams S-324 and S-526 generate more steam than is needed for heating. The excess could be diverted to offset some power requirements. This was not explored in this analysis due to the expected limited impact in the face of extreme electricity requirements.

Cooling Efficiency of HX-401

The extreme amount of cooling water required for HX-401 represents a great cause for concern, and it is likely that a heat exchanger is not the most effective medium. Alternative cooling configurations such as a cooling tower should be explored before implementation.

Solar Heating

Solar Salt is traditionally heated in large solar fields. The current process uses a solar salt furnace as suggested by Table 22.32 of PPDP. If a solar heating setup is feasible given the conditions in Brazil, this would save construction of one furnace and allow for the combustion gases currently used in that furnace to be diverted elsewhere. The cost would be the construction of a second storage tank and other units needed for the solar heating process. More information can be found in Appendix D.
Section V
Unit Descriptions
V. UNIT DESCRIPTIONS

Section 000: Input Storage & Clarification

Storage Tanks
Base Purchase Cost: $1,906,800

At desired flow rate of 1.25 million pounds per hour of molasses, fifteen storage tanks are necessary to ensure that production can continue 330 days per year. Since the vapor pressure of molasses is extremely low, cone-roof tanks made of carbon steel were appropriate. The molasses is stored at ambient temperature, 77°F, and atmospheric pressure, 14.7 psia. Each tank is 20,000,000 gallons, which is the upper limit of construction according (p.589, PPDP). The storage tanks are expected to operate at 76% capacity with a residence time of six days. For the nine months of the year that molasses produced, five tanks will be used to allow for deliveries once monthly. Since molasses is unavailable approximately 92 days per year, the remaining ten tanks will be filled as shortly as possible before end of season. Each tank empties on a rotating basis into stream S-000. See SC-000 for calculations.

Pumps
P-000
Base Purchase Cost: $84,300

This is a centrifugal cast iron pump that adds a driving force of 2 psi to the molasses feed, S-000, drawing it from the storage tank in operation and introducing it to the clarification process. This satisfies Heuristic 38 of PPDP, which allows for a 2 psi pressure drop across 100 ft of pipe. The electricity required is 2.23 kW. The pump head is 3.89 ft.

Other Equipment
C-000
Base Purchase Cost: $1,255,988
This unit is a clarifier vessel. Diluted molasses enters the clarifier to allow particles to settle. It handles 58,838 gallons per minute of liquid overflow. It has a settling area of 88,258 square feet and a diameter of 335 feet. It is made of concrete. It has a rotating rake to collect the sludge that accumulates at the bottom.

**F-000**
Base Purchase Cost: $129,978

This unit is a rotary drum filter. It removes 1500 pounds of filtrate per day per square foot. It has a surface area of 115 square feet.

**Section 100: Hydrolysis**

**Pumps**

**P-100, P-101, P-102**
Base Purchase Cost: $10,200

This is a centrifugal pump, of 304 stainless steel, that pumps the three identically split streams of input from SPT-100 to HX-100, HX-101, and HX-102. It operates at a rate of 5,610 ft$^3$/hr. The energy requirement for the pump is 14.13 HP. The pump operates at an efficiency of 0.74. The pump head is 50.1 ft. The pressure change across the pump is 1.75 atm.

**P-103, P-104, P-105**
Base Purchase Cost: $179,700

This is a centrifugal pump, of 304 stainless steel, that pumps the three identical streams from R-100, R-101, and R-102 to HX-200. It operates at a rate of 5,785 ft$^3$/hr. The energy requirement for the pump is 659.10 HP. The pump operates at an efficiency of 0.74. The pump head is 2,342.5 ft. The pressure change across the pump is 1167 psi.
Heat Exchangers

HX-100, HX-101, HX-102
Base Purchase Cost: $51,200

This is a heat exchanger that is used to heat the sucrose and water feed to R-100, R-101, and R-102 and cool the product from the condensation reaction. This is a floating head shell and tube heat exchanger. The streams exiting pumps P-100, P-101, and P-102 are passed through the heat exchangers at a flow rate of 5,610 ft³/hr. The temperature of the cold inlet stream is increased from 77°F to 212°F (25°C to 100°C). The hot inlet stream from SPT-400 is passed through the heat exchangers at a flow rate of 276,000 ft³/hr. The temperature of the hot inlet stream is decreased from 698°F to 506°F (370°C to 263.3°C). The heat duty of heat exchanger is 36,902,766 BTU/hr. The heat transfer area is 1,615 ft². Both the shell side and the tube side are made of 304 stainless steel.

Reactors

R-100, R-101, R-102
Base Purchase Cost: $175,600

This is a reactor used to convert the sucrose and water fed into it from P-100, P-101, and P-102 to glucose and water. The reactor is fed at 5,994 ft³/hr. The reactor operates at 100°C and 1 atm. It is a 304 stainless steel fixed bed reactor loaded with catalyst. It has a capacity of 6,309 ft³/hr. The weight of the catalyst needed per charge is 147,000,000 g, costing approximately $2,490,000 discounted to $0.621 million at 25%. The reactor is 23 feet tall and has a 6 ft diameter.

Catalyst

CAT-100
Base Purchase Cost, including Lifetime Recharge: 6,388,200

The catalyst used in hydrolysis is an HY-faujasite catalyst with an SI/Al ratio of 15. This is a zeolite catalyst much in the same sense as others that are needed later. This catalyst is used as a means to speed up the hydrolysis of sucrose in water which if just let to sit would take years to
Castillo, Ernst, Lerch, Winchester

hydrolyze into glucose. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.

To create the catalyst H₄SiO₄ is fed into Na₂AlO₂ in a ratio of approximately 12 to 1. The catalyst is then steam-aged, for 2 hours at 500°C to create the stable faujasite crystals. Once the faujasite crystals have been obtained (NH₄)₂SiF₆ is added as desired until the specified Si/Al ratio is reached. The deactivation of this catalyst is estimated to be 13.29 grams of catalyst / lbmol of reactant fed, based on an estimate for a similar catalyst. This estimate may be a little high for the deactivation however seeing as the catalyst did not lose any activity in the 7 day period of testing (Moreau, 1999). It is also known that the catalyst can easily be regenerated a limited number of times by using a thermal technique of burning off the coked particles by passing a stream of hot (500°C) air through the catalyst.

To calculate the costs of the catalyst market pricing for H₄SiO₄, Na₂AlO₂, and (NH₄)₂SiF₆ were obtained. Once that was completed using data from Moreau, 1999, the weight hourly space velocity (WHSV) was calculated to be approximately 1.93 hr⁻¹. Using the value of the WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 147,000,000 grams of catalyst per charge. From this it is known that to achieve a 15 to 1 ration of Si to Al that a ratio of 12:1:3 of H₄SiO₄: Na₂AlO₂: (NH₄)₂SiF₆ is needed to achieve this goal. So to determine the overall pricing of the catalyst 147,000,000 was multiplied by 12/16 and the market price of H₄SiO₄ per gram and added to 147,000,000 multiplied by 1/16 and the market price of Na₂AlO₂ per gram and 147,000,000 multiplied by 3/16 and the market price of (NH₄)₂SiF₆ per gram. This yields a value of $2.49 million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.62 million per charge.
The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 24,169 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $3.52 million and with the discount 25% bulk pricing $0.88 million. See SC-C00 for calculations.

Section 200: Hydrogenation

Pumps

P-200, P-201, P-202, P-203, P-204, P-205
Base Purchase Cost: $6,500

This is a centrifugal pump, of 304 stainless steel, that pumps the six identically split streams from SPT-200 to R-200, R-201, R-202, R-203, R-204, and R-205. It operates at a rate of 2,828 ft$^3$/hr. The energy requirement for the pump is 0.61 HP. The pump operates at an efficiency of 0.68. The pump head is 3.9 ft. The pressure change across the pump is 2 psi.

P-206, P-207, P-208, P-209, P-210, P-211
Base Purchase Cost: $6,500

This is a centrifugal pump, of 304 stainless steel, that pumps the six identical streams from R-200, R-201, R-202, R-203, R-204, and R-205 to MIX-200. It operates at a rate of 2,841 ft$^3$/hr. The energy requirement for the pump is 0.61 HP. The pump operates at an efficiency of 0.68. The pump head is 3.9 ft. The pressure change across the pump is 2 psi.

Heat Exchangers
Castillo, Ernst, Lerch, Winchester

HX-200
Base Purchase Cost: $286,600

This is a heat exchanger that is used to cool the glucose and water stream going to SPT-200 by using cooling water. This is a floating head shell and tube heat exchanger. The stream exiting MIX-100 is passed through the heat exchanger at a flow rate of 17,739 ft³/hr. The temperature of the hot inlet stream is decreased from 214.16°F to 173.75°F (101.2°C to 78.75°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 20,654 ft³/hr. The temperature of the cold inlet stream is increased from 90°F to 120°F (32.2°C to 48.9°C). The heat duty of heat exchanger is 40,777,165 BTU/hr. The heat transfer area is 9057 ft². Both the shell side and the tube side are made of 304 stainless steel.

Reactors
R-200, R-201, R-202, R-203, R-204, R-205
Base Purchase Cost: $191,300

This is a reactor used to convert the glucose fed into it from P-200, P-201, P-202, P-203, P-204, and P-205 to sorbitol. The reactor is fed at 2,828 ft³/hr. The reactor operates at 353K and 80 bar. It is a Teflon coated stainless steel 316 trickle bed reactor loaded with catalyst. It is a Teflon coated reactor to prevent catalyst poisoning. It has a capacity of 211,083 lb/hr. The weight of the catalyst needed per charge is 24,202,200 g, costing approximately $47.5 million discounted to $11.9 million at 25%. The reactor is 18.5 feet tall and has a 5 ft diameter.

Catalyst
CAT-200
Purchase Cost, including Lifetime Recharge: $15,391,100

In typical glucose hydrogenation Ni used to be the preferred catalyst metal because of its high activity and low costs. Unfortunately Ni catalysts can leach and have their activity decreased rapidly and require possibly expensive separation processes to purify the product of the Ni particles. Ru catalysts however don’t suffer from the same drawbacks as Ni which makes it much more appealing.
Section V: Unit Descriptions

as a commercial catalyst. The catalyst which yielded the best result for glucose hydrogenation was a Ru05Ai catalyst.

The Ru05Ai catalyst creation process would be prepared by the impregnation of Al₂O₃ with Ruthenium (III) Acetylacetonate. The Al₂O₃ is used as the support metal for the activation of the ruthenium. To begin the preparation of the catalyst 73 g Al₂O₃ is mixed with 150 ml of toluene and stirred for 15 minutes. Once the Al₂O₃/toluene slurry is prepared, 2.907 g Ruthenium (III) Acetylacetonate is dissolved in a separate 150 ml of toluene and this solution is added to the slurry. This new slurry is stirred for one hour while being swirled occasionally to homogenize it. The toluene is also left to evaporate at room temperature at this time. The catalyst is then heated in by a helium stream within four hours to 250°C and held at this temperature for two more hours. To reduce the catalyst it is heated to 350°C within one hour by a hydrogen stream and held at this temperature for three more hours. (Kusserow, 2002) However based on the cost of buying of the raw materials needed and additional labor costs needed for creating the catalyst it was found to be much cheaper to purchase a catalyst that is believed to be similar from a supplier. Catalyst deactivation was assumed to be seven years because of Ruthenium’s use as a precious metal. It was also assumed that the catalyst could be sold back to the supplier for half of the purchase price.

To estimate the cost of making the catalyst, the prices of Ruthenium (III) Acetyl Acetonate, Al₂O₃, and toluene were obtained. A scale up factor was determined based on the volumetric flow rate of the reactant feed and the volume of catalyst added. The scale up factor (SUF) is merely the volumetric flow rate of the limiting reactant feed needed divided by 0.04 L and 7.5 (a “volumetric hourly space velocity”). Based on a 300ml:73g:2.907g ratio of Toluene: Al₂O₃:Ruthenium (III) Acetyl Acetonate the price of the catalyst was determined to be $229.7 million. With the discount to 25% it would cost $57.4 million. Unfortunately these prices were too high so a similar catalyst that could be bought from a supplier was searched for. To determine the mass of the catalyst needed to
be purchased the wt% of Ru in Ruthenium (III) Acetyl Acetonate was determined (approximately 25.4%). Using this value and the mass of Ruthenium (III) Acetyl Acetonate needed it was determined that 1.21 million grams of Ru would be needed. Using the catalyst specification of 5% Ru it was found that 24.2 million grams of catalyst is needed. To purchase this much catalyst from the supplier it was found to cost $47.5 million much less than the amount of money to produce it. Using the discount 25%, the price drops to $11.9 million. See calculation SC-C01.

Section 300: Aqueous Phase Reforming

Pumps

P-300
Base Purchase Cost: $8,500

This is a centrifugal pump, of 304 stainless steel, that pumps the heated sorbitol stream from HX-300 to HX-301. It operates at a rate of 4,859 ft³/hr. The energy requirement for the pump is 3.39 HP. The pump operates at an efficiency of 0.73. The pump head is 14.4 ft. The pressure change across the pump is 7 psi.

P-301
Base Purchase Cost: $5,200

This is a centrifugal pump, of 304 stainless steel, that pumps the recycled sorbitol stream from F-300 to MIX-300. It operates at a rate of 1,390 ft³/hr. The energy requirement for the pump is 0.34 HP. The pump operates at an efficiency of 0.60. The pump head is 4.5 ft. The pressure change across the pump is 2 psi.

P-302
Base Purchase Cost: $8,400

This is a centrifugal pump, of 304 stainless steel, that pumps the mixed sorbitol stream from MIX-300 to HX-300. It operates at a rate of 4,784 ft³/hr. The energy requirement for the pump is
2.39 HP. The pump operates at an efficiency of 0.73. The pump head is 10.2 ft. The pressure change across the pump is 5 psi.

**Heat Exchangers**

**HX-300**

Base Purchase Cost: $56,000

This is a heat exchanger that is used to cool the hydrogen, carbon dioxide, alkane, and water stream from VAL-301, while heating the mixed sorbitol stream from P-302. This is a floating head shell and tube heat exchanger. The stream exiting VAL-301 is passed through the heat exchanger at a flow rate of 6,364,400 ft$^3$/hr. The temperature of the hot inlet stream is decreased from 338.74°F to 273.58°F (170.4°C to 134.2°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 4784 ft$^3$/hr. The temperature of the cold inlet stream is increased from 227.58°F to 253.58°F (108.7°C to 123.1°C). The heat duty of heat exchanger is 7,700,625 BTU/hr. The heat transfer area is 2,422 ft$^2$. Both the shell side and the tube side are made of 304 stainless steel.

**HX-301**

Base Purchase Cost: $174,200

This is a heat exchanger that is used to heat the mix sorbitol stream from P-300 using some of the heat generated from the furnace. This is a floating head shell and tube heat exchanger. The stream exiting P-300 is passed through the heat exchanger at a flow rate of 4,858 ft$^3$/hr. The temperature of the cold inlet stream is increased from 253.59°F to 359.6°F (123.1°C to 182°C). The heat duty of heat exchanger is 32,547,633 BTU/hr. The heat transfer area is 8505 ft$^2$. Both the shell side and the tube side are made of 304 stainless steel.

**HX-302**

Base Purchase Cost: $16,000

This is a heat exchanger that is used to cool the hydrogen stream from HX-400 using cooling water. This is a floating head shell and tube heat exchanger. The stream exiting HX-400 is passed
through the heat exchanger at a flow rate of 25,003 ft³/hr. The temperature of the hot inlet stream is decreased from 254.1°F to 173.75°F (123.4°C to 78.75°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 1003 ft³/hr. The temperature of the cold inlet stream is increased from 90°F to 120°F (32.2°C to 48.9°C). The heat duty of heat exchanger is 2,014,133 BTU/hr. The heat transfer area is 157 ft². Both the shell side and the tube side are made of 304 stainless steel.

**HX-303**

Base Purchase Cost: $185,100

This is a heat exchanger that is used to cool the hydrogen, carbon dioxide, alkane, and water stream from HX-300 using chilled water. This is a floating head shell and tube heat exchanger. The stream exiting HX-300 is passed through the heat exchanger at a flow rate of 5,840,540 ft³/hr. The temperature of the hot inlet stream is decreased from 273.5°F to 140°F (134.2°C to 60°C). The cold inlet stream is passed through the heat exchangers at a flow rate of 22,258 ft³/hr. The temperature of the cold inlet stream is increased from 40°F to 120°F (4.4°C to 48.9°C). The heat duty of heat exchanger is 122,304,595 BTU/hr. The heat transfer area is 12,179 ft². Both the shell side and the tube side are made of 304 stainless steel.

**Reactors**

**R-300**

Base Purchase Cost: $231,800

This is a reactor used to convert the sorbitol fed into it from HX-301 to hydrogen, alkanes, and carbon dioxide. The reactor is fed at 5,209 ft³/hr. The reactor operates at 182°C and 50 bar. It is a 304 stainless steel trickle bed reactor loaded with catalyst. It has a capacity of 6,309 ft³/hr. The weight of the catalyst needed per charge is 44,266,068 g, costing approximately $240.9 million discounted to $60.2 million at 25%. The reactor is 22 feet tall and has a 6 ft diameter.
Separators

SEP-300
Base Purchase Cost: $52,000

This is a separator used to separate hydrogen from carbon dioxide and alkanes. It utilizes pressure swing adsorption technology to create the separation. The separator is fed with 3,414,410 ft³/hr. The separator is 12 ft tall and has a diameter of 11.5 ft. The separator has a heat duty of -14,767,649 BTU/hr. The separator is made of 304 stainless steel.

ST-300
Base Purchase Cost: $344,890

This unit is a horizontal pressure vessel for the storage of hydrogen gas. At 77°F and 20 bar, the tank can hold 3393 cubic feet of hydrogen. The storage tank is constructed from carbon steel. It is 30 feet long and has a diameter of 12 feet.

ADS-300, ADS-301, ADS-302, ADS-303
Base Purchase Cost: $477,000

This unit is an adsorption column for pressure swing adsorption. It is 35 feet high and has a diameter of 8 feet. Gas feed enters the column at 20 bar. It is filled with 81,000 pounds of zeolite 13x.

F-300
Base Purchase Cost: $35,100

This is a separator used to separate sorbitol from hydrogen, carbon dioxide, and alkanes. It utilizes flash vaporization technology to create the separation. The separator is fed with 255,086 ft³/hr. The separator is 13 ft tall and has a diameter of 6 ft. The separator has a heat duty of 77,018,428 BTU/hr. The separator operates at 359.6°F and 20 bar. The separator is made of 304 stainless steel.
F-301
Base Purchase Cost: $34,600

This is a separator used to separate water from hydrogen, carbon dioxide, and alkanes. It utilizes flash vaporization technology to create the separation. The separator is fed with 2,739,570 ft³/hr. The separator is 12 ft tall and has a diameter of 9.5 ft. The separator has a heat duty of 5,106,795 BTU/hr. The separator operates at 140°F and 1 atm. The separator is made of 304 stainless steel.

Compressors
CMP-300
Base Purchase Cost: $10,132,800

This is a multi stage compressor, of 304 stainless steel, used to compress the hydrogen from SEP-300 to 80 bar. It operates at a rate of 1,612,640 ft³/hr. The energy requirement for the compressor is 22,340 HP. The net cooling duty of the compressor is -30,562,822 BTU/hr. The pressure change across the compressor is 1149.6 psi.

Catalyst
CAT-300
Purchase Cost, including Lifetime Recharging: $77,995,500

The catalyst presentation in the patent was presented independent of the operating conditions discussion. The catalyst chosen is an RhReCe catalyst. The catalyst was made by adding 3.86g of Rhodium(III) Nitrate, 1.64g of Perrhenic acid, and 2.21g of Cerium(III) Nitrate hexahydrate to 12 ml of deionized water in the presence of titania modified carbon and dried overnight under a vacuum at 100°C. The titania modified carbon was created by adding 1.95g of Titanium n-butoxide to 12 ml of anhydrous isopropanol in the presence of 10g of activated carbon. However due to the high costs of Rhodium (III) Nitrate it was assumed that the metals were purchased at market price and could be sold back to the supplier after deactivation for half the purchase price to be regenerated. It was also assumed that because rhodium is a precious metal the deactivation would take place over 7 years.
To calculate the price of this catalyst the prices of Rhodium (III) Nitrate, Perrhenic acid, and Cerium (III) Nitrate were obtained. It necessary that 175,659 lb of sorbitol is fed to the APR reactor per hour and from the specified WHSV of 1.8 (WO 2007/075476) it was determined that 97,588 lb (or 44.27 million grams) of catalyst is needed. Since 17.985 g is needed per batch the number of batches needed to be made is 2.46 million. The price of each material per batch was determined by the mass needed of each per batch and the price of the material. These prices were multiplied by the number of batches needed and summed together. This returns a value of $686 million which is entirely unreasonable. So to combat this issue the market prices of the metals themselves was obtained and the weight of each metal needed per batch was determined using weight percents. The price of each metal was converted to a per gram basis and the value of a single batch was determined to be $72.25 for 13.28 grams. The mass of catalyst needed was divided by the 13.28 and multiplied the $72.25 to determine the value of the catalyst needed by metal market pricing. This returned a more reasonable, although still very expensive, $240.9 million per charge. Using the discount to 25%, the price becomes $60.2 million. See calculation SC-C02.

Section 400: Condensation

**Pumps**

**P-400**

FOB Cost: $119,300

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-400 to heat exchanger HX-402. It operates at a temperature of 204 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 1727 gallons per minute with a density of 72.33 lb/ft³. The pump head is 3.98 feet. The pump uses 1.86kW of electricity and generates 2.5hp of brake power operating at 80.8% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.
Castillo, Ernst, Lerch, Winchester

**P-401**

FOB Cost: $272,300

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-404 the splitter SPT-400. It operates at a temperature of 698 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 2818 gallons per minute with a density of 44.33 lb/ft$^3$. The pump head is 6.5 feet. The pump uses 2.94kW of electricity and generates 3.94hp of brake power operating at 83.5% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

**P-402**

FOB Cost: $121,400

This unit is a centrifugal pump made of carbon steel. It pumps sorbitol from heat exchanger HX-404 the heat exchanger HX-404. It operates at a temperature of 302 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 1832 gallons per minute with a density of 68.18 lb/ft$^3$. The pump head is 4.33 feet. The pump uses 1.96kW of electricity and generates 2.63hp of brake power operating at 81.1% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

**Heat Exchangers:**

**HX-400**

FOB Cost: $764,100

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by heating 1 million lb/hr sorbitol from 177 to 204 degrees Fahrenheit and cooling 7420lb/hr hydrogen from 1150 to 254 degrees Fahrenheit. It transfers a heat duty of 23.23 million BTU/hr over 1340 ft$^2$ of heat transfer area and was designed assuming an overall heat coefficient of 50 BTU/hr-ft$^2$-°F. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified
Section V: Unit Descriptions

minimum temperature approach of 50 degrees Fahrenheit, and a specified hot/cold outlet
temperature approach of 50 degrees Fahrenheit to reasonably maximize heat transfer.

**HX-401**
FOB Cost: $1,375,300

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by cooling 1 million lb/hr condensation product from 414 to 122 degrees Fahrenheit and using 29.652 million lb/hr cooling water heated from 90 to 120 degrees Fahrenheit. It transfers a heat duty of 978.49 million BTU/hr over 55,302 ft² of heat transfer area and was designed assuming an overall heat coefficient of 150 BTU/hr-ft²-o°F. It is 20 ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 20 degrees Fahrenheit, and a specified hot stream outlet temperature 122 degrees Fahrenheit as required for the three-phase separation.

**HX-402**
FOB Cost: $1,375,300

This is a shell and tube heat exchanger made of carbon steel on the tube side and 304 stainless steel on the shell side. It performs heat recovery by heating 1 million lb/hr condensation product from 204 to 206 degrees Fahrenheit and cooling 74508 lb/hr xylenes from 276 to 226 degrees Fahrenheit. It transfers a heat duty of 1.805 million BTU/hr over 1084 ft² of heat transfer area and was designed assuming an overall heat coefficient of 40 BTU/hr-ft²-o°F. It is 20 ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 20 degrees Fahrenheit, and a specified hot/cold outlet temperature approach of 20 degrees Fahrenheit in order to reasonably assure maximum heat transfer.

**HX-403**
FOB Cost: $762,600
Castillo, Ernst, Lerch, Winchester

This is a shell and tube heat exchanger made of carbon steel. It performs heat recovery by heating 1 million lb/hr of sorbitol solution from 207 to 302 degrees Fahrenheit and cooling 214929 lb/hr of transalkylation product from 850 to 352 degrees Fahrenheit. It transfers a heat duty of 83.72 million BTU/hr over 6890 ft$^2$ of heat transfer area and was designed assuming an overall heat coefficient of 40 BTU/hr-ft$^2$-°F. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 50 degrees Fahrenheit, and a specified hot/cold outlet temperature approach of 50 degrees Fahrenheit in order to reasonably assure maximum heat transfer.

HX-404
FOB Cost: $11,854,500

This is a shell and tube heat exchanger made of carbon steel. It heats 1 million lb/hr sorbitol solution from 640 to 698 degrees Fahrenheit using hot Dowtherm A. It transfers a heat duty of 527.76 million BTU/hr over 2858 ft$^2$ of heat transfer area. It is 20ft long. The above was calculated by ASPEN based on the specified outlet temperature of the sorbitol necessary for condensation.

Reactors
R-400, R-401, R-402, R-403
FOB Cost: $460,500 each

These are packed bed reactors made of carbon steel responsible for the catalyzed condensation reactor that convert sorbitol into para-xylene and other aromatics. Four identical reactors are used due to size limitations. Each reactor handles 250480 pounds of sorbitol solution per hour and operates at a temperature of 698 degrees Fahrenheit. Each has a volume of 4759.2 gallons, of which 3331 is working volume. Each is 22.5 feet high and 6 feet in diameter.

CAT-400
Purchase Cost, including Lifetime Reloading: $11,745,000
An activated zeolite or aluminosilicate catalyst, normally pentasil (more commonly called ZSM-5), facilitates the reaction. Zeolites have a porous structure that can accommodate a wide variety of cations. The cations are loosely held and exchange easily with cations in the contacted solution. Similar catalysts are used in the aqueous phase reforming and transalkylation portions of this process, and information on their manufacture and properties can be found in US patent 2008/0300435 A1. For the condensation of sorbitol to produce para-xylene, ZSM-5, with a thirty-to-one silicon dioxide to aluminum oxide ratio, is treated with a gallium nitrate solution, dried overnight in a vacuum oven, and subsequently calcined in flowing air at 400 degrees Celsius to effect 1.2% loading by weight of gallium (Example 46 in the patent). The WHSV is specified in the patent as 2 hr⁻¹. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.

To calculate the same costs of the catalyst market pricing for $H_4SiO_4$ and $Na_2AlO_2$ were used. Using the value of the specified WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 120.2 million grams of catalyst per charge. From this, it is known that to achieve a 30 to 1 ration of Si to Al which implies that a ratio of 30:1 of $H_4SiO_4$:$Na_2AlO_2$ is needed to achieve this goal. So to determine the overall pricing of the catalyst, 120.2 million was multiplied by 30/31 and the market price of $H_4SiO_4$ per gram and added to 120.2 million multiplied by 1/31 and the market price of $Na_2AlO_2$ per gram. This yields a value of $2.41 million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.60 million per charge.

The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a
result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 38,674 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $6.80 million and with the discount 25% bulk pricing $1.70 million. See calculation SC-C03.

Section 500: Separations

**P-500**
FOB Cost: $45,200

This unit is a centrifugal pump made of carbon steel. It pumps bottoms product from column DC-500 to column DC-501. It operates at a temperature of 346 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 407 gallons per minute with a specific gravity of 0.773. The pump head is 5.98 feet. The pump operates at 68.4% efficiency, uses 0.47kW of electricity and generates 0.63hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

**DP-500**
FOB Cost: $9,900

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-500 back into the column DC-500 or out. It operates at a temperature of 259 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 494 gallons per minute with a specific gravity of 0.773. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

**P-501**
FOB Cost: $53,600

This unit is a centrifugal pump made of carbon steel. It pumps organic condensation product from the three phase separator (SEP-500) to the first column (DC-500). It operates at a temperature of 250 degrees Fahrenheit. It moves 524 gallons per minute with a specific gravity of 0.777. The
pump head is 5.98 feet. The pump operates at 70.9% efficiency, uses 0.585kW of electricity and
generates 0.78hp of brake power. These properties were determined using ASPEN for the specified
2psi pressure increase.

**DP-501**
FOB Cost: $13,600

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-501 back
into the column or out. It operates at a temperature of 326 degrees Fahrenheit. It moves 864 gallons
per minute with a specific gravity of 0.758. The pump operates at 70% efficiency. These properties
were determined automatically by ASPEN as part of the RADFRAC subroutine.

**P-502**
FOB Cost: $53,500

This unit is a centrifugal pump made of carbon steel. It pumps bottoms product from column
DC-502 in a recycle loop back to column DC-500. It operates at a temperature of 289 degrees
Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 489 gallons
per minute with a specific gravity of 0.776. The pump head is 5.95 feet. The pump operates at 70.2%
efficiency, uses 0.55kW of electricity and generates 0.74hp of brake power. These properties were
determined using ASPEN for the specified 2psi pressure increase.

**DP-502**
FOB Cost: $26,600

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-502 back
into the column or out. It operates at a temperature of 250 degrees Fahrenheit. It moves 2105 gallons
per minute with a specific gravity of 0.776. The pump operates at 70% efficiency. These properties
were determined automatically by ASPEN as part of the RADFRAC subroutine.

**P-503**
FOB Cost: $34,000
This unit is a centrifugal pump made of carbon steel. It pumps distillate from column DC-502 to column DC-503. It operates at a temperature of 70 degrees Fahrenheit and provides a specified 2psi increase to combat frictional losses. It moves 176 gallons per minute with a specific gravity of 0.775. The pump head is 5.96 feet. The pump operates at 59.3% efficiency, uses 0.23kW of electricity and generates 0.31hp of brake power. These properties were determined using ASPEN for the specified 2psi pressure increase.

**DP-503**

FOB Cost: $6,200

This unit is a centrifugal pump made of carbon steel. It pumps distillate from DC-503 back into the column or out. It operates at a temperature of 250 degrees Fahrenheit. It moves 183 gallons per minute with a specific gravity of 0.812. The pump operates at 70% efficiency. These properties were determined automatically by ASPEN as part of the RADFRAC subroutine.

**Heat Exchangers:**

**RB-500**

FOB Cost: $381,200

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 18984 ft$^2$ and heat duty of 75.4 million BTU/hr.

**RB-501**

FOB Cost: $238,100

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 11149 ft$^2$ and heat duty of 44.5 million BTU/hr.
Section V: Unit Descriptions

**RB-502**
FOB Cost: $313,700

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inchitch, with tube outside diameter 1 in. It have heat transfer area of 15247 ft$^2$ and heat duty of 146.8 million BTU/hr.

**RB-503**
FOB Cost: $29,600

This is a shell and tube heat exchanger made of carbon steel which heat and boil fractions of the bottoms product of its respective distillation columns so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It have heat transfer area of 998 ft$^2$ and heat duty of 16.5 million BTU/hr.

**CND-500**

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 1639 ft$^2$.

**CND-501**

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 1585 ft$^2$.

**CND-502**

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has
Castillo, Ernst, Lerch, Winchester

tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 13760 ft\(^2\).

**CND-503**

This is a shell and tube heat exchanger made of carbon steel which condenses fractions of the distillate of its respective distillation column so that the material can reenter the column. Each has tube length of 20 feet, a triangular-shaped 1.25 inch itch, with tube outside diameter 1 in. It has heat transfer area of 18473 ft\(^2\).

**Columns**

**DC-500**

**FOB Cost:** $528,900

This is a distillation tower separating toluene in the light key from para-xylene in the heavy key. The distillate is sent to transalkylation for further conversion, while the bottoms is further distilled to isolate xylenes. The tower has tangent-to-tangent height 68 feet and diameter 16.5 feet, in included 28 trays spaced 2 feet apart. The column operates with a reflux ratio of 0.809, is fed on tray 15, and has an average tray efficiency 0.58. The operating temperature is 296 degrees Fahrenheit. 96% of the light key and 8% of the heavy key were recovered in the distillate.

**DC-501**

**FOB Cost:** $458,000

This is a distillation tower separating xylenes in the light key from isopropylbenzene in the heavy key. The distillate is sent to crystallization for further para-xylene isolation, while the bottoms is burned in the furnace. The tower has tangent-to-tangent height 94 feet and diameter 12.5 feet, in included 41 trays spaced 2 feet apart. The column operates with a reflux ratio of 3.0, is fed on tray 16, and has an average tray efficiency 0.64. The operating temperature is 332 degrees Fahrenheit. 96% of the light key and 17% of the light key were recovered in the distillate.
DC-502
FOB Cost: $580,000

This is a distillation tower separating benzene in the light key from toluene in the heavy key. The distillate is sent to column DC-503 to isolate benzene, while the bottoms is recycled for further recovery of xylenes. The tower has tangent-to-tangent height 48 feet and diameter 22.5 feet, in included 18 trays spaced 2 feet apart. The column operates with a reflux ratio of 12, is fed on stage 15, and has an average tray efficiency 0.56. The operating temperature is 239 degrees Fahrenheit. 98% of the light key and 1% of the heavy key were recovered in the distillate.

DC-503
FOB Cost: $117,600

This is a distillation tower separating alkanes in the light key from benzene in the heavy key. The distillate is burned in the furnace, while the bottoms sold for profit. The tower has tangent-to-tangent height 48 feet and diameter 22.5 feet, in included 18 trays spaced 2 feet apart. The column operates with a reflux ratio of 3, is fed on stage 16, and has an average tray efficiency 0.49. The operating temperature is 176 degrees Fahrenheit. 99% of the light key and 4% of the light key were recovered in the distillate.

Drums:

AD-500
FOB Cost: $27,700

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 3022 gallons and diameter of 17 feet.

AD-501
FOB Cost: $35,100

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 5089 gallons and diameter of 20.5 feet.

AD-502
Casillo, Ernst, Lerch, Winchester
FOB Cost: $51,600

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 13326 gallons and diameter of 28 feet.

AD-503
FOB Cost: $18,700

This is a carbon steel horizontal drum which handles the accumulated condensate from the condenser of the column. It has a volume of 1128 gallons and diameter of 12 feet.

Section 600: Transalkylation

Pumps
P-601
FOB Cost: $54,200

This is a centrifugal carbon steel pump which pumps sorbitol solution from heat exchanger HX-601 to mixer MIX-502. It operates at 182 degrees Fahrenheit and moves 85780 lb/hrr of fluid with density 48.5 lb/ft³. The pump generates a pressure increase of 2psi to combat frictional losses. The pump head is 5.9 feet. The pump uses 0.67kW of electricity and generates 0.89hp of brake power operating at 72.2% efficiency. These properties were determined using ASPEN for the specified 2psi pressure increase.

Heat Exchangers
HX-600
FOB Cost: $541,900

This is a shell and tube heat exchanger made of 304 stainless steel. It heats 214922 lb/hr of toluene-rich distillate from DC-500 from 209 to 850 degrees Fahrenheit using molten salt. It transfers a heat duty of 71.35 million BTU/hr. It is 20ft long. The above was calculated by ASPEN based on the specified outlet temperature of the sorbitol necessary for condensation.

HX-601
FOB Cost: $119,400
This is a shell and tube heat exchanger made of carbon steel. It cools 2406 lb/hr transalkylation product from 352 to 182 degrees Fahrenheit using 568330 lb/hr of cooling water heated from 90 to 120 Fahrenheit. It transfers a heat duty of 18.59 million BTU/hr over 1536 ft\(^2\) of heat transfer area and was designed assuming an overall heat coefficient of 80 BTU/hr-ft\(^2\)-°F. It is 20ft long. The above was calculated by ASPEN based on the assumed overall heat transfer coefficient, a specified minimum temperature approach of 50 degrees Fahrenheit, and a specified hot stream outlet temperature of 182 degrees Fahrenheit, suitable for entry into DC-502.

**Reactors**

**R-600**

FOB Cost: $567,800

This is a low alloy steel packed-bed catalytic reactor that hosts the transalkylation reaction, converting toluene into saleable para-xylene and benzene. The reactor handles 214922 pounds of feed per hour and operates at a temperature of 850 degrees Fahrenheit. It has a volume of 9254 gallons, of which 6477 gallons is working volume. It is 28 feet tall and 7.5 feet in diameter.

**CAT-600**

Purchase Cost, including Lifetime Reloading: $6,065,700

Transalkylation is catalyzed by zeolite catalyst, similar to the catalyzed condensation. In Example 2 of US Patent 6323381, a “selectivated large crystal HZSM-5 was used.” This catalyst has a Si/Al ratio of 70 to 1. Although no further specifics were given, the catalyst was assumed similar enough to the condensation catalyst that both could be ordered together in order to achieve economies of scale. Information and assumptions applied to pricing for the condensation catalyst were also applied to the transalkylation catalyst. To make up for the relatively rapid deactivation of the catalyst it possible to add a column of new catalyst to continuously pump catalyst into the reactor while filtering out older catalyst.
To calculate the same costs of the catalyst market pricing for $\text{H}_4\text{SiO}_4$ and $\text{Na}_2\text{AlO}_2$ were used. Using the data given in the patent, and the assumption that the feed was 100% toluene a WHSV of $5.2 \text{ hr}^{-1}$ was determined. Using this value for WHSV and the known amount of feed to the reactor, the amount of catalyst needed was determined to be 12.6 million grams of catalyst per charge. From this, it is known that to achieve a 30 to 1 ration of Si to Al which implies that a ratio of 70:1 of $\text{H}_4\text{SiO}_4$: $\text{Na}_2\text{AlO}_2$ is needed to achieve this goal. So to determine the overall pricing of the catalyst, 12.6 million was multiplied by $70/71$ and the market price of $\text{H}_4\text{SiO}_4$ per gram and added to 12.6 million multiplied by $1/71$ and the market price of $\text{Na}_2\text{AlO}_2$ per gram. This yields a value of $0.25$ million per charge. It was then assumed to have a discount to 25% for bulk pricing options which gives a value of $0.06$ million per charge.

The estimated deactivation of the catalyst, 13.29 grams/lbmol reactant was used to determine the deactivation of the catalyst. Since the flow rate of the reactant is known to determine the amount of deactivated catalyst in an hour the hourly lbmol flow rate is multiplied by 13.29. This yields a result of grams of deactivated catalyst per hour. The hourly deactivation of catalyst is 20,883 grams per hour. The price of the hourly deactivated catalyst is determined via the same process as before and this value is multiplied by 24 hours and 365 days to get a yearly cost. The cost was determined to be $3.67$ million and with the discount 25% bulk pricing $0.92$ million. See calculation SC-C04.

**Section 700: Furnace & Heating Cycles**

**Storage Tanks**

**ST-700**

FOB Cost: $719,833

ST-700 is a spherical pressure vessel for the storage of Dowtherm A, as part of the Dowtherm A heating cycle. To store 532,000 pounds of Dowtherm A with a residence time of six minutes and a capacity usage of 70%, a tank volume of 124,000 gallons is required. Low-alloy steel
is an appropriate material since the heating fluid is stored saturated at 698°F and 93.69 psia. See SC-701 for volume and pricing calculations for storage vessels.

**ST-701**

**FOB Cost:** $658,751

This unit is a cone-roof tank for the storage of Solar Salt, as part of the molten salt heating cycle. With a suggested residence time of six hours and capacity usage of 70%, the tank has a volume of 639,300 gallons. The heating fluid is stored at 900°F and 3 psig. Due to the high operating temperature, the tank must be constructed from stainless steel. See SC-701 for calculations.

**Furnaces**

**FRN-700**

**FOB Cost:** $3,253,196

This unit is a stainless steel molten salt fired heater, which provides the heat for the molten salt heating cycle. An inlet stream of molten salt, S-723, absorbs 62 MBtu/h from this furnace and increases 200 degrees in temperature to 1100°F. This temperature rise is suggested by the materials specifications for Solar Salt (Appendix D) and 900°F is selected as the lower bound because it is the lowest temperature that does not violate the requirements of HX-600. Heuristic 26 of PPDP suggests a minimum approach temperature for fired heaters of flue temperature 250°F above inlet. Therefore, the air intake (S-705) is adjusted to 26,000 lbmol/h such that the flue gas (S-706) exits at 1150°F. Fortunately, this temperature is below the maximum and above the minimum suggested by PPDP Heuristic 30, which allows complete combustion and avoids any condensation. However, the extreme conditions require stainless steel, rather than carbon steel. The furnace operates at atmospheric pressure. See SC-702 for pricing calculations.

**FRN-701, FRN-702**

**FOB Cost:** $5,186,584
Castillo, Ernst, Lerch, Winchester

About 532 MBtu/h of Dowtherm A latent heat is required to heat the condensation inlet stream, S-405, to 698°F. Since the upper limit of heat transfer on commercial fired heaters is 340 MBtu/h (p.482, PPDP), two Dowtherm A furnaces are required for this phase-change process. Although close to the upper limit, carbon steel furnaces are acceptable in this range of operating temperatures (Appendix 23, PPDP). Again following Heuristic 26 of PPDP, an air intake of about 135,000 lbmol/h is specified to ensure the flue gas leaves at 1000°F. The furnaces operate at atmospheric pressure. See SC-702 for pricing calculations.

FRN -703
FOB Cost: $1,495,615

This carbon steel steam boiler provides the steam for heating units RB-500, RB-501, RB-502, RB-503, HX-301, and WC-500. The total energy required from this steam is 319 MBtu/h, and it is provided by evaporating and condensing water from stream S-526. The furnace operates at 405°F and 260 psig in order to provide steam at the pressure required for HX-301, which is the maximum. An air flow rate of 290,000 lbmol/h sets the flue gas exit temperature at about 500°F, which satisfies Heuristic 26 (PPDP). See SC-702 for pricing calculations.

Pumps
P-700, P-701
FOB Cost: $481,700

This is a centrifugal pump Dowtherm A loop that operates at a rate of 8517 gpm. The energy required is 7.84 kW, given an efficiency of 0.859. This provides 79.13 ft of head with a pressure increase of 23.5 psi. This pressure increase was specified to satisfy Heuristic 38, which allows for a pressure drop due to liquid flow through 100 ft of pipe; and Heuristic 31, which dictates a 20 psi allowance for drop through a furnace and a 1.5 psi drop for phase changes in a heat exchanger (PPDP).

P-702
FOB Cost: $854,100

120
This is a centrifugal pump in the Dowtherm A loop that operates at a rate of 16111 gpm. The energy required is 29.65 kW, given an efficiency of 0.859. This provides 12.74 ft of head with a pressure increase of 4 psi. This pressure increase was specified to satisfy Heuristic 38 (PPDP), which allows for a pressure drop due to liquid flow through 100 ft of each of two pipes, after splitting.

P-703
FOB Cost: $114,000
This is a centrifugal pump in the molten salt loop that operates at a rate of 2599 gpm. The energy required is 60.98 kW, given an efficiency of 0.826. This provides 163.80 ft of head with a pressure increase of 70.5 psi. This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP), while also increasing the flow to operating pressure of 50 psig from 3 psig. Note that molten salts are not available in ASPEN and this pump was sized using milk as an estimate since the viscosities of milk and Solar Salt are within a few millipoise of each other.

P-704
FOB Cost: $94,100
This is a centrifugal pump in the molten salt loop that operates at a rate of 2560 gpm. The energy required is 2.49 kW, given an efficiency of 0.826. This provides 4.65 ft of head with a pressure increase of 2 psi. This pressure increase was specified to satisfy Heuristic 38 (PPDP). Note that molten salts are not available in ASPEN and this pump was sized using milk as an estimate since the viscosities of milk and Solar Salt are within a few millipoise of each other.

P-705(IN), P-705(IN)-2
FOB Cost: $4,500
This is a centrifugal pump in the HX-301 steam loop that operates at a rate of 88 gpm. The energy required is 0.14 (0.21) kW, given an efficiency of 0.506. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

P-706(IN)
FOB Cost: $5,200
This is a centrifugal pump in the RB-500 steam loop that operates at a rate of 192 gpm. The energy required is 0.25 (0.38) kW, given an efficiency of 0.604. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

**P-707(IN)**

FOB Cost: $4,700

This is a centrifugal pump in the RB-501 steam loop that operates at a rate of 118 gpm. The energy required is 0.17 (0.26) kW, given an efficiency of 0.545. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

**P-708(IN)**

FOB Cost: $6,300

This is a centrifugal pump in the RB-502 steam loop that operates at a rate of 354 gpm. The energy required is 0.47 (0.63) kW, given an efficiency of 0.671. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).

**P-709(IN)**

FOB Cost: $4,300

This is a centrifugal pump in the RB-503 steam loop that operates at a rate of 38 gpm. The energy required is 0.08 (0.12) kW, given an efficiency of 0.385. This provides 4.68 (7.02) ft of head with a pressure increase of 2 psi (3 psi). This pressure increase was specified to satisfy Heuristics 31 and 38 (PPDP).
Section VI
Specification Sheets
### VI. SPECIFICATION SHEETS

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>P-100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>No. Req’d</td>
<td></td>
<td>3</td>
</tr>
</tbody>
</table>

**Function**

Overcome frictional losses from the beginning of the process.

**Operation**

Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-101</th>
<th>Exit: S-104</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>415000</td>
</tr>
<tr>
<td>Temperature(°F)</td>
<td>77</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
</tr>
<tr>
<td>Sucrose</td>
<td>207500</td>
</tr>
<tr>
<td>Water</td>
<td>207500</td>
</tr>
</tbody>
</table>

**Design Data:**

- Density of Fluid (lb/cuft): 73.97
- Brake Power (hp): 14.13
- Pump Head (ft): 50.1
- Electricity Requirements (kW): 10.54
- Material of Construction: 304 Stainless Steel

**Cost, C_P, C_TDC**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost, C_P</td>
<td>$10,200</td>
</tr>
<tr>
<td>Cost, C_TDC</td>
<td>$57,500</td>
</tr>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
</tr>
</tbody>
</table>
## Heat Exchanger

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>HX-100</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>No. Req'd</td>
<td></td>
<td>3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Function</th>
<th>Cool condensation product while heating sucrose and water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operation</td>
<td>Continuous</td>
</tr>
</tbody>
</table>

### Materials Handled:

<table>
<thead>
<tr>
<th>Materials Handled</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td></td>
<td>S-417</td>
<td>S-420</td>
</tr>
</tbody>
</table>

| Quantity (lb/hr)  | 333972     | 333972     | 415000     | 415000      |
| Temperature (°F)  | 698        | 506        | 77         | 212         |
| Composition (lb/hr) |           |            |            |             |
| p-Xylene         | 13808      | 13808      | 0          | 0           |
| o-Xylene         | 256        | 256        | 0          | 0           |
| m-Xylene         | 28         | 28         | 0          | 0           |
| n-Butane         | 2033       | 2033       | 0          | 0           |
| n-Pentane        | 7795       | 7795       | 0          | 0           |
| n-Hexane         | 10845      | 10845      | 0          | 0           |
| Water            | 266130     | 266130     | 207500     | 207500      |
| Hydrogen         | 130        | 130        | 0          | 0           |
| Sucrose          | 0          | 0          | 207500     | 207500      |
| Ethylbenzene     | 142        | 142        | 0          | 0           |
| Toluene          | 3050       | 3050       | 0          | 0           |
| Benzene          | 678        | 678        | 0          | 0           |
| Naphthalene      | 6778       | 6778       | 0          | 0           |
| 1,2,4-trimethylbenzene | 6778   | 6778       | 0          | 0           |
| isopropylbenzene | 10168      | 10168      | 0          | 0           |
| n-Heptane        | 2372       | 2372       | 0          | 0           |
| 1-Butene         | 326        | 326        | 0          | 0           |
| 1-Pentene        | 985        | 985        | 0          | 0           |
| 1-Hexene         | 1370       | 1370       | 0          | 0           |
| 1-Heptene        | 300        | 300        | 0          | 0           |

### Design Data:

<table>
<thead>
<tr>
<th>Heat Duty (BTU):</th>
<th>36,902,756</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall Heat Coefficient (BTU/h)</td>
<td>50</td>
</tr>
<tr>
<td>Heat Transfer Area (ft²):</td>
<td>1,615</td>
</tr>
<tr>
<td>Type:</td>
<td>Floating Head</td>
</tr>
<tr>
<td>Material of Construction:</td>
<td>Shell: Carbon Steel</td>
</tr>
<tr>
<td></td>
<td>Tube: 304 Stainless Steel</td>
</tr>
</tbody>
</table>

### Cost, C_{PB}, C_{TDC}:

| Utilities: | $51,200 | $226,000 |
| Comments:  |        |         |
# Reactor

## Identification
- Item: R-200
- Item No: 200
- No. Req’d: 6

## Function
- Convert Glucose to Sorbitol
- Continuous

## Materials Handled:

<table>
<thead>
<tr>
<th>Material</th>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-211</td>
<td>S-317</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>207498</td>
<td>1236</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>176</td>
<td>176</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Glucose</td>
<td>98289</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>1236</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>109209</td>
<td>0</td>
</tr>
</tbody>
</table>

## Design Data:
- Volume (gal): 2717.45
- Working Vol initial (L): 7200
- Working Vol at end (L): 7200
- Height (ft): 18.5
- Diameter (ft): 5
- Material of Construction: Teflon Coated Stainless Steel

## Cost, $C_{PB}, C_{TDC}$:
- $191,300$
- $348,800$

## Utilities:

## Comments:
<table>
<thead>
<tr>
<th>Identification</th>
<th>R-300</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>300</td>
</tr>
<tr>
<td>No. Req'd</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function Operation**: Converts Sorbitol to Hydrogen, Carbon Dioxide, and Propane. Continuous.

**Materials Handled**:

<table>
<thead>
<tr>
<th></th>
<th>S-305</th>
<th>S-306</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>339323</td>
<td>339323</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>359.6</td>
<td>359.6</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>89</td>
<td>93769</td>
</tr>
<tr>
<td>Propane</td>
<td>13.5</td>
<td>28191</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.5</td>
<td>7421</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>175660</td>
<td>43128</td>
</tr>
<tr>
<td>Water</td>
<td>163560</td>
<td>166814</td>
</tr>
</tbody>
</table>

**Design Data**:

- Volume (gal): 4653.45
- Working Vol initial (L): 12329
- Working Vol at end (L): N/A
- Height (ft): 22
- Diameter (ft): 6
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**: $231,800, $405,000

**Utilities**: 

**Comments**: 

## Reactor

### Identification
- Item: R-100
- Item No: 100
- No. Req’ed: 3

### Function
- Convert Sucrose and Water to Glucose
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-107</td>
<td>S-110</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>415000</td>
<td>415000</td>
</tr>
<tr>
<td><strong>Temperature(°F)</strong></td>
<td>212</td>
<td>212</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Glucose</td>
<td>0</td>
<td>218420</td>
</tr>
<tr>
<td>Sucrose</td>
<td>207500</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>207500</td>
<td>196580</td>
</tr>
</tbody>
</table>

### Design Data:
- Volume (gal): 4864.97
- Working Vol initial (L): 12890
- Working Vol at end (L): 12890
- Height (ft): 23
- Diameter (ft): 6
- Material of Construction: 304 Stainless Steel

### Cost, C<sub>PB</sub>, C<sub>TDC</sub>:
- $179,100
- $338,600

### Utilities:

### Comments:
<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-103</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Item No: 100</td>
</tr>
<tr>
<td></td>
<td>No. Req’d 3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Function Operation</th>
<th>Increase pressure of glucose and water stream to 80 bar Continuous</th>
</tr>
</thead>
</table>

| Materials Handled: |
|-------------------|------------------|------------------|------------------|
|                   | Feed: S-110     | Exit: S-113      |
| Quantity (lb/hr)  | 415000           | 415000           |
| Temperature(°F)   | 212              | 214.16           |
| Composition (lb/hr) | 218420       | 218420           |
| Glucose           |                  |                  |
| Water             | 196580           | 196580           |

| Design Data: | Density of Fluid (lb/ft³): 71.74 |
|              | Brake Power (hp): 659.11 |
|              | Pump Head (ft): 2342.5 |
|              | Electricity Requirements (kW): 491.5 |
|              | Material of Construction: 304 Stainless Steel |

<table>
<thead>
<tr>
<th>Cost, C_PB, C_TDC</th>
<th>$179,700</th>
<th>$284,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Section VI: Specification Sheets

#### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-200</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>200</td>
</tr>
<tr>
<td>No. Req'd</td>
<td>6</td>
</tr>
</tbody>
</table>

**Function**
- Bring the glucose and water stream to the hydrogenation reactor.

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-200</th>
<th>Exit: S-211</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>207498</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>173.75</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Glucose 109209</td>
</tr>
<tr>
<td></td>
<td>Water</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/ft³): 73.37
- Brake Power (hp): 0.61
- Pump Head (ft): 3.9
- Electricity Requirements (kW): 0.45
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**
- $6,500
- $52,800

**Utilities:**
- Electricity

**Comments:**

### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-206</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td>206</td>
</tr>
<tr>
<td>No. Req'd</td>
<td>6</td>
</tr>
</tbody>
</table>

**Function**
- To bring the sorbitol and water stream to the stream mixer.

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-212</th>
<th>Exit: S-218</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>208734</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>173.75</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Sorbitol 110440</td>
</tr>
<tr>
<td></td>
<td>Water</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/ft³): 73.47
- Brake Power (hp): 0.61
- Pump Head (ft): 3.9
- Electricity Requirements (kW): 0.45
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**
- $6,500
- $52,800

**Utilities:**
- Electricity

**Comments:**
### Pump

**Identification**
- Item: P-300
- Item No: 300
- No. Req’d: 1

**Function**
To bring the mixed sorbitol stream to a heat exchanger for heat. Continuous

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-303</th>
<th>Exit: S-304</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>339323</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>253.57</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>339323</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>175660</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.5</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>89</td>
</tr>
<tr>
<td>Propane</td>
<td>13.5</td>
</tr>
<tr>
<td>Water</td>
<td>163560</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/cuft): 69.84
- Brake Power (hp): 3.39
- Pump Head (ft): 14.4
- Electricity Requirements (kW): 2.53
- Material of Construction: 304 Stainless Steel

**Cost, C_{FB} - C_{TCO}**
- $8,500
- $57,900

**Utilities:**
- Electricity

**Comments:**

---

### Pump

**Identification**
- Item: P-301
- Item No: 301
- No. Req’d: 1

**Function**
To bring the sorbitol recycle to the sorbitol mixer. Continuous

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-308</th>
<th>Exit: S-309</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>88840</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>359.6</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>43128</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0.5</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>89</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>13.5</td>
</tr>
<tr>
<td>Water</td>
<td>45609</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/cuft): 63.92
- Brake Power (hp): 0.34
- Pump Head (ft): 4.5
- Electricity Requirements (kW): 0.25
- Material of Construction: 304 Stainless Steel

**Cost, C_{FB} - C_{TCO}**
- $5,200
- $39,500

**Utilities:**
- Electricity

**Comments:**
## Section VI: Specification Sheets

### Pump

<table>
<thead>
<tr>
<th><strong>Identification</strong></th>
<th><strong>Item:</strong></th>
<th><strong>P-302</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Item No:</strong></td>
<td>302</td>
<td></td>
</tr>
<tr>
<td><strong>No. Req’d:</strong></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Function**

- Bring the mixed sorbitol stream to a heat exchanger for heat.

**Operation**

- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-301</th>
<th>Exit: S-302</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>3393.23</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>227.58</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>1756.60</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.5</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>89</td>
</tr>
<tr>
<td>Propane</td>
<td>13.5</td>
</tr>
<tr>
<td>Water</td>
<td>1635.60</td>
</tr>
</tbody>
</table>

**Design Data:**

- Density of Fluid (lb/ft³): 70.93
- Brake Power (hp): 2.39
- Pump Head (ft): 10.2
- Electricity Requirements (kW): 1.78
- Material of Construction: 304 Stainless Steel

**Cost, $C_{PB}$, $C_{TDC}$:** $8,400 / $57,700

**Utilities:** Electricity

**Comments:**

### Heat Exchanger

<table>
<thead>
<tr>
<th><strong>Identification</strong></th>
<th><strong>Item:</strong></th>
<th><strong>HX-200</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Item No:</strong></td>
<td>200</td>
<td></td>
</tr>
<tr>
<td><strong>No. Req’d:</strong></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Function**

- Cool glucose and water to hydrogenation reactor temperature

**Operation**

- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th><strong>Shell Side</strong></th>
<th><strong>Tube Side</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream In: S-119</td>
<td>Stream Out: S-225</td>
</tr>
<tr>
<td>1245000</td>
<td>1245000</td>
</tr>
<tr>
<td>Stream In: CW-100</td>
<td>Stream Out: CW-101</td>
</tr>
<tr>
<td>214.15</td>
<td>175.73</td>
</tr>
<tr>
<td>90</td>
<td>120</td>
</tr>
</tbody>
</table>

**Design Data:**

- Heat Duty (BTU): 40,777,165
- Overall Heat Coefficient (BTU/h)
- Heat Transfer Area (ft²): 9,057
- Type: Floating Head
- Material of Construction: Shell: 304 Stainless Steel
  - Tube: 304 Stainless Steel

**Cost, $C_{PB}$, $C_{TDC}$:** $286,600 / $485,300

**Utilities:** Cooling Water

**Comments:**
<table>
<thead>
<tr>
<th>Heat Exchanger</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Function</strong></td>
</tr>
<tr>
<td><strong>Operation</strong></td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td><strong>Shell Side</strong></td>
</tr>
<tr>
<td>Stream In: S-311</td>
</tr>
<tr>
<td>Stream In: S-302</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
</tr>
<tr>
<td>Sorbitol</td>
</tr>
<tr>
<td>Propane</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
</tr>
<tr>
<td>Water</td>
</tr>
<tr>
<td>Hydrogen</td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td>Heat Duty (BTU)</td>
</tr>
<tr>
<td>Overall Heat Coefficient (BTU/h)</td>
</tr>
<tr>
<td>Heat Transfer Area (ft²):</td>
</tr>
<tr>
<td>Type: Floating Head</td>
</tr>
<tr>
<td>Material of Construction</td>
</tr>
<tr>
<td>Shell: 304 Stainless Steel</td>
</tr>
<tr>
<td>Tube: 304 Stainless Steel</td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td><strong>Cost, ( C_{PB}, C_{TDC} ):</strong></td>
</tr>
<tr>
<td><strong>Comments:</strong></td>
</tr>
</tbody>
</table>
# Heat Exchanger

**Identification**
- Item: HX-301
- Item No: 301
- No. Req’d: 1

**Function**
To heat mixed sorbitol stream to APR reactor temperature.

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td>S-304</td>
<td>S-305</td>
</tr>
</tbody>
</table>

| Quantity (lb/hr) | 339323 | 339323 |
| Temperature (°F) | 253.59 | 359.6 |

<table>
<thead>
<tr>
<th>Composition (lb/hr)</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>175660</td>
<td>175660</td>
</tr>
<tr>
<td>Propane</td>
<td>13.5</td>
<td>13.5</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>89</td>
<td>89</td>
</tr>
<tr>
<td>Water</td>
<td>163560</td>
<td>163560</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU): 32,547,633
- Overall Heat Coefficient (BTU/hr): 50
- Heat Transfer Area (ft²): 8,505
- Type: Floating Head
- Material of Construction
  - Shell: 304 Stainless Steel
  - Tube: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}:**
- $174,200
- $335,000

**Utilities:**

**Comments:** Heat from furnace used
### Heat Exchanger

**Identification**
- Item: HX-302
- Item No: 302
- No. Req'd: 1

**Function**
- To cool hydrogen to hydrogenation reactor temperature.
- Operation: Continuous

<table>
<thead>
<tr>
<th>Materials Handled</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream In</td>
<td>Stream Out</td>
<td>Stream In</td>
</tr>
<tr>
<td>S-315</td>
<td>S-316</td>
<td>CW-300</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>7420</td>
<td>7420</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>254.16</td>
<td>173.75</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>7420</td>
<td>7420</td>
</tr>
<tr>
<td>Hydrogen</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU): 2,014,133
- Overall Heat Coefficient (BTU/°F): 120
- Heat Transfer Area (ft²): 157
- Type: Floating Head
- Material of Construction:
  - Shell: 304 Stainless Steel
  - Tube: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}:**
- $16,000
- $33,100

**Utilities:** Cooling Water

**Comments:**

---

### Heat Exchanger

**Identification**
- Item: HX-303
- Item No: 303
- No. Req'd: 1

**Function**
- To cool hydrogen to be fed to the compressor.
- Operation: Continuous

<table>
<thead>
<tr>
<th>Materials Handled</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream In</td>
<td>Stream Out</td>
<td>Stream In</td>
</tr>
<tr>
<td>S-312</td>
<td>S-326</td>
<td>CW-304</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>250488.38</td>
<td>250488.38</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>273.58</td>
<td>140</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>0.38</td>
<td>0.38</td>
</tr>
<tr>
<td>Sulfur</td>
<td>28178</td>
<td>28178</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>93680</td>
<td>93680</td>
</tr>
<tr>
<td>Water</td>
<td>121210</td>
<td>121210</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7420</td>
<td>7420</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU): 122,304,595
- Overall Heat Coefficient (BTU/°F): 80
- Heat Transfer Area (ft²): 12,256
- Type: Floating Head
- Material of Construction:
  - Shell: 304 Stainless Steel
  - Tube: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}:**
- $185,100
- $347,600

**Utilities:** Chilled Water

**Comments:**

---

136
### Section VI: Specification Sheets

#### Compressor

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:CMP-300</th>
<th>Item No.:300</th>
<th>No. Req'd:1</th>
</tr>
</thead>
</table>

**Function** Compress hydrogen to hydrogenation reactor pressure. **Operation** Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-325</th>
<th>Exit: S-314</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>7420</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>140</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Hydrogen</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/ft³): 0.0046014
- Total Work (hp): 22340
- Outlet Pressure (psia): 1164.3
- Net Cooling Duty (Btu/hr): -30,562,822
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**
- $10,132,800
- $10,868,300

**Utilities:**
- Electricity
- Cooling Water

**Comments:**

#### Separator

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:SEP-300</th>
<th>Item No.:300</th>
<th>No. Req'd:1</th>
</tr>
</thead>
</table>

**Function** Assure swing adsorption to remove hydrogen from other gas. **Operation** Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-323</td>
<td>S-313</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>407409</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>140</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Propane</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>93678</td>
</tr>
<tr>
<td>Water</td>
<td>24541</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7420</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (Btu/hr): -14,767,649
- Height (ft): 12
- Diameter (ft): 11.5
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**
- $52,000
- $202,700

**Utilities:**

**Comments:**

---

137
### Separator

#### Identification
- Item: F-300
- Item No: 300
- No. Req’d: 1

#### Function
- Operation: To separate unreacted sorbitol from APR products.
- Continuous

#### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Streams In</th>
<th>Streams Out</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-307</td>
<td>S-308</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>339319</td>
<td>88840</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>314.62</td>
<td>359.6</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>43128</td>
<td>43128</td>
</tr>
<tr>
<td>Propane</td>
<td>28191</td>
<td>13.5</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>93769</td>
<td>89</td>
</tr>
<tr>
<td>Water</td>
<td>166810</td>
<td>45609</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7421</td>
<td>0.5</td>
</tr>
</tbody>
</table>

#### Design Data:
- Heat Duty (BTU/hr): 77,018,428
- Height (ft): 13
- Diameter (ft): 6
- Material of Construction: 304 Stainless Steel

#### Cost, C_{PB}, C_{TDC}:
- $35,100
- $142,900

#### Utilities:

#### Comments:
### Separator

**Identification**
- Item: F-301
- Item No.: 301
- No. Req'd: 1

**Function**
- To separate water from the APR products to be fed into PSA

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td>S-326</td>
<td>S-324</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>250488.38</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>140</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Sorbitol: 0.38</td>
</tr>
<tr>
<td></td>
<td>Propane: 28178</td>
</tr>
<tr>
<td></td>
<td>Carbon Dioxide: 53680</td>
</tr>
<tr>
<td></td>
<td>Water: 12120</td>
</tr>
<tr>
<td></td>
<td>Hydrogen: 7420</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU/hr): 5,106,795
- Height (ft): 12
- Diameter (ft): 9.5
- Material of Construction: 304 Stainless Steel

**Cost, C_{PE}, C_{TDC}:**
- $34,600
- $157,400

**Utilities:**

**Comments:**

---

### Pump

**Identification**
- Item: P-400
- Item No.: 400
- No. Req'd: 1

**Function**
- To pump the sorbitol water stream from HX-400 to HK-402

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-402</th>
<th>Exit: S-403</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>1001930</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>204</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Sorbitol: 530120</td>
</tr>
<tr>
<td></td>
<td>Water: 471810</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/cuft): 72.33
- Brake Power (hp): 2.5
- Pump Head (ft): 3.98
- Electricity Requirements (kW): 1.86
- Material of Construction: Carbon Steel

**Cost, C_{PE}, C_{TDC}**
- $10,600
- $119,300

**Utilities:**
- Electricity

**Comments:**

---

139
### Pump

**Identification**

<table>
<thead>
<tr>
<th>Item</th>
<th>Item No.</th>
<th>No. Req'd</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-401</td>
<td>401</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function**

To pump the sorbitol water stream from HX-404 to SPT-400

**Operation**

Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-406</th>
<th>Exit: S-407</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>1001930</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>698.1</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>530120</td>
</tr>
<tr>
<td>Water</td>
<td>471810</td>
</tr>
</tbody>
</table>

**Design Data:**

- Density of Fluid (lb/cuft): 44.33
- Brake Power (hp): 3.94
- Pump Head (ft): 6.5
- Electricity Requirements (kW): 2.94
- Material of Construction: Carbon Steel

**Cost, C_{PB}, C_{T0C}**

<table>
<thead>
<tr>
<th>Electricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$13,400</td>
</tr>
</tbody>
</table>

**Utility:**

Electricity

**Comments:**

---

### Pump

**Identification**

<table>
<thead>
<tr>
<th>Item</th>
<th>Item No.</th>
<th>No. Req'd</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-402</td>
<td>402</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function**

To pump the sorbitol water stream from HX-403 to HX-404

**Operation**

Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Feed: S-404</th>
<th>Exit: S-405</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>1001930</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>302</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>530120</td>
</tr>
<tr>
<td>Water</td>
<td>471810</td>
</tr>
</tbody>
</table>

**Design Data:**

- Density of Fluid (lb/cuft): 68.18
- Brake Power (hp): 2.63
- Pump Head (ft): 4.33
- Electricity Requirements (kW): 1.96
- Material of Construction: Carbon Steel

**Cost, C_{PB}, C_{T0C}**

<table>
<thead>
<tr>
<th>Electricity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$11,000</td>
</tr>
</tbody>
</table>

**Utility:**

Electricity

**Comments:**
Section VI: Specification Sheets

### Heat Exchanger

**Identification**
- Item: HX-400
- Item No: 400
- No. Req'd: 1

**Function**
To heat the fresh sorbitol and cool hydrogen.

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td></td>
<td>S-314</td>
<td>S-315</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>7420</td>
<td>7420</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>1150</td>
<td>254</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Sorbitol</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>Hydrogen</td>
<td>7420</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU): 23,227,907
- Overall Heat Coefficient (BTU/hr): 50
- Heat Transfer Area (ft²): 1,340
- Type: Floating Head
- Material of Construction:
  - Shell: 304 Stainless Steel
  - Tube: Carbon Steel

**Cost, C_{PB}, C_{TDC}:**
- $156,900
- $764,100

**Utilities:**

**Comments:**
# Heat Exchanger

**Identification**
- Item: HX-401
- Item No: 401
- No. Req'd: 1

**Function**
- To heat the fresh sorbitol and cool hydrogen.

**Operation**
- Continuous

## Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>1001939</td>
<td>90</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>414</td>
<td>122</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>41424</td>
<td>0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>769</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>85</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>6101</td>
<td>0</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>23386</td>
<td>0</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>32537</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>798400</td>
<td>29652000</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>392</td>
<td>392</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>427</td>
<td>427</td>
</tr>
<tr>
<td>Toluene</td>
<td>9151</td>
<td>9151</td>
</tr>
<tr>
<td>Benzene</td>
<td>2033</td>
<td>2033</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>20336</td>
<td>20336</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20336</td>
<td>20336</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>30503</td>
<td>30503</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>7117</td>
<td>7117</td>
</tr>
<tr>
<td>1-Butene</td>
<td>979</td>
<td>979</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>2954</td>
<td>2954</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>4110</td>
<td>4110</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>899</td>
<td>899</td>
</tr>
</tbody>
</table>

## Design Data:
- Overall Heat Coefficient (BTU/hr): 150
- Heat Transfer Area (ft²): 55,302
- Type: Floating Head
- Material of Construction:
  - Shell: 304 Stainless Steel
  - Tube: Carbon Steel

**Cost, C_P, C_TCE:**
- $834,400
- $1,375,300

**Utilities:**
- Cooling Water

**Comments:**
### Heat Exchanger

**Identification**
- Item: HX-402
- Item No: 402
- No. Req’d: 1

**Function**
- Operation: Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Stream In</th>
<th>Stream Out</th>
<th>Stream In</th>
<th>Stream Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shell Side</td>
<td>Tube Side</td>
<td>Shell Side</td>
<td>Tube Side</td>
</tr>
<tr>
<td>S-507</td>
<td>S-403</td>
<td>S-520</td>
<td>S-426</td>
</tr>
</tbody>
</table>

- **Quantity (lb/hr)**
  - S-507: 74508, S-403: 1001930
  - S-520: 74508, S-426: 1001930

- **Temperature (°F)**
  - S-507: 276, S-403: 204
  - S-520: 226, S-426: 206

- **Composition (lb/hr)**
  - Sorbitol: 0
  - p-Xylene: 53936
  - o-Xylene: 2490
  - m-Xylene: 5216
  - Water: 0
  - Ethylbenzene: 877
  - Toluene: 6745
  - 1,2,4-Trimethylbenzene: 60
  - Isopropylbenzene: 5184

**Design Data:**
- Heat Duty (BTU): 1,804,692
- Overall Heat Coefficient (BTU/°F): 40
- Heat Transfer Area (ft²): 1,084
- Type: Floating Head
- Material of Construction:
  - Shell: Carbon Steel
  - Tube: Carbon Steel

**Cost, $C_{PB}, C_{TDC}: $39,400, $136,400**

**Utilities:**

**Comments:**
# Heat Exchanger

## Identification
- **Item:** HX-403
- **Item No:** 403
- **No. Req’d:** 1

## Function
- **Operation:** To heat the fresh sorbitol and cool the transalkylation product
  - Continuous

## Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th></th>
<th>Tube Side</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stream In:</td>
<td>Stream Out:</td>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td></td>
<td>S-601</td>
<td>S-602</td>
<td>S-426</td>
<td>S-404</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>214929</td>
<td>214929</td>
<td>1001930</td>
<td>1001930</td>
</tr>
<tr>
<td><strong>Temperature(°F)</strong></td>
<td>850</td>
<td>352</td>
<td>207</td>
<td>302</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
<td></td>
<td>530120</td>
<td>530120</td>
</tr>
<tr>
<td>Sorbitol</td>
<td>0</td>
<td>0</td>
<td>530120</td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>19973</td>
<td>19973</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2909</td>
<td>2909</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5817</td>
<td>5817</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2613</td>
<td>2613</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16082</td>
<td>16082</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
<td>471810</td>
<td>471810</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>581</td>
<td>581</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>143500</td>
<td>143500</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>21137</td>
<td>21137</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1931</td>
<td>1931</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

## Design Data:
- **Heat Duty (BTU):** 83,722,732
- **Overall Heat Coefficient (BTU/hr):** 40
- **Heat Transfer Area (ft²):** 6,890

**Type:** Floating Head  
**Material of Construction:**  
- Shell: Carbon Steel  
- Tube: Carbon Steel

## Cost, C_{PB}, C_{TDC}:
- **$383,200**  
- **$762,600**

## Utilities:

## Comments:
## Heat Exchanger

### Identification
- Item: HX-404
- Item No: 404
- No. Req’d: 1

### Function
- Operation: heat fresh sorbitol stream to condensation reactor temperature
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th>Materials</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream In:</td>
<td>Stream Out:</td>
<td>Stream In:</td>
</tr>
<tr>
<td>S-405</td>
<td>S-406</td>
<td></td>
</tr>
</tbody>
</table>

| Quantity (lb/hr) | 1001930  | 1001930  |
| Temperature (°F) | 253.59   | 359.6    |
| Composition (lb/hr) |          |          |
| Sorbitol        | 530120   | 530120   |
| Water           | 471810   | 471810   |

### Design Data:
- Heat Duty (BTU): 527,756,123
- Overall Heat Coefficient (BTU/h): 50
- Heat Transfer Area (ft²): 138,719
- Type: Floating Head
- Material of Construction:
  - Shell: Carbon Steel
  - Tube: Carbon Steel

### Cost, $C_{PB}$, $C_{TDC}$:
- $3,568,600
- $11,854,500

### Utilities:

### Comments:
<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: R-400</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>400</td>
</tr>
<tr>
<td>No. Req'd</td>
<td>4</td>
</tr>
</tbody>
</table>

**Function**
Convert Sorbitol to Aromatics and other Hydrocarbons

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Streams In:</th>
<th>S-408</th>
<th>S-412</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>250480</td>
<td>250480</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>698</td>
<td>698</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sorbitol</td>
<td>132530</td>
<td>0</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>0</td>
<td>10357</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>0</td>
<td>193</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>0</td>
<td>22</td>
</tr>
<tr>
<td>n-Butane</td>
<td>0</td>
<td>1526</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>0</td>
<td>5847</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>0</td>
<td>8135</td>
</tr>
<tr>
<td>Water</td>
<td>117950</td>
<td>199604</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0</td>
<td>98</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0</td>
<td>107</td>
</tr>
<tr>
<td>Toluene</td>
<td>0</td>
<td>2288</td>
</tr>
<tr>
<td>Benzene</td>
<td>0</td>
<td>508</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0</td>
<td>5085</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0</td>
<td>5085</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>0</td>
<td>7627</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>0</td>
<td>1780</td>
</tr>
<tr>
<td>1-Butene</td>
<td>0</td>
<td>225</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>0</td>
<td>740</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>0</td>
<td>1028</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>0</td>
<td>225</td>
</tr>
</tbody>
</table>

**Design Data:**

| Volume (gal): | 4753.21 |
| Working Vol initial (L): | 12610 |
| Working Vol at end (L): | 12610 |
| Height (ft): | 22.5 |
| Diameter (ft): | 6 |
| Material of Construction: | Carbon Steel |

**Cost, C<sub>PB</sub>, C<sub>TDC</sub>:**

<table>
<thead>
<tr>
<th>Utilities:</th>
<th>$233,300</th>
</tr>
</thead>
<tbody>
<tr>
<td>$460,500</td>
<td>----------</td>
</tr>
</tbody>
</table>

**Comments:**

---

146
## Section VI: Specification Sheets

### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th></th>
<th>P-500</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No.</td>
<td></td>
<td>500</td>
<td></td>
</tr>
<tr>
<td>No. Req'd</td>
<td></td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

### Function
Pumps bottoms from DC-500 as feed for DC-501.

### Operation
Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th>Feed: S-505</th>
<th>S-506</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>29976</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>296</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>56067</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>3549</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5484</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>890</td>
</tr>
<tr>
<td>Toluene</td>
<td>6745</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>20320</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20254</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>23976</td>
</tr>
</tbody>
</table>

### Design Data:
- Density of Fluid (lb/ft³): 48.25
- Brake Power (hp): 0.63
- Pump Head (ft): 5.97
- Electricity Requirements (kW): 0.47
- Material of Construction: Carbon Steel

### Cost, C<sub>PC</sub>, C<sub>TDC</sub>
- $6,600
- $45,200

### Utilities:
- Electricity

### Comments:
<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-501</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>501</td>
</tr>
<tr>
<td>No. Req’d</td>
<td>1</td>
</tr>
</tbody>
</table>

**Function**
Pumps hydrocarbons from SEP-500 to MIX-500.

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-501</th>
<th>S-502</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>29976</td>
<td>29976</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>122</td>
<td>122</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>56067</td>
<td>56067</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>3543</td>
<td>3543</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5484</td>
<td>5484</td>
</tr>
<tr>
<td>n-Butane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n-Hexane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>890</td>
<td>890</td>
</tr>
<tr>
<td>Toluene</td>
<td>6745</td>
<td>6745</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>20320</td>
<td>20320</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20254</td>
<td>20254</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>29976</td>
<td>29976</td>
</tr>
</tbody>
</table>

**Design Data:**

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-501</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of Fluid (lb/cuft):</td>
<td>61.61</td>
</tr>
<tr>
<td>Brake Power (hp):</td>
<td>0.78</td>
</tr>
<tr>
<td>Pump Head (ft):</td>
<td>5.93</td>
</tr>
<tr>
<td>Electricity Requirements (kW):</td>
<td>0.59</td>
</tr>
<tr>
<td>Material of Construction:</td>
<td>Carbon Steel</td>
</tr>
</tbody>
</table>

**Cost, C_{PB}; C_{TDC}**

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-501</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost $</td>
<td>$6,600</td>
</tr>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
</tr>
<tr>
<td>Cost $</td>
<td>$45,200</td>
</tr>
<tr>
<td>Material of Construction:</td>
<td>Carbon Steel</td>
</tr>
</tbody>
</table>
### Section VI: Specification Sheets

#### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>P-502</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>502</td>
</tr>
<tr>
<td>No. Req’d</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Function**

- Pumps bottoms from DC-502 to MIX-500.
- Continuous

**Operation**

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-513</th>
<th>S-514</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>172681</td>
<td>172681</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>239</td>
<td>239</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>19973</td>
<td>19973</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2909</td>
<td>2909</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>5817</td>
<td>5817</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>582</td>
<td>582</td>
</tr>
<tr>
<td>Toluene</td>
<td>142675</td>
<td>142675</td>
</tr>
<tr>
<td>Benzene</td>
<td>725</td>
<td>725</td>
</tr>
</tbody>
</table>

**Design Data:**

- Density of Fluid (lb/ft³): 45.46
- Brake Power (hp): 0.74
- Pump Head (ft): 5.94
- Electricity Requirements (kW): 0.55
- Material of Construction: Carbon Steel

**Cost, Cₚₑ, Cₑₑₜ:**

- $7,200
- $53,500

**Utilities:**

- Electricity

**Comments:**
# Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>P-503</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>503</td>
</tr>
<tr>
<td>No. Req’d</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Function Operation</th>
<th>Cumps distillate from DC-502 after it passes through HX-500 to DC-50</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Materials Handled:</th>
<th>Feed: S-501</th>
<th>S-502</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>61987</td>
<td>61987</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>62.8</td>
<td>62.8</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2614</td>
<td>2614</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16183</td>
<td>16183</td>
</tr>
<tr>
<td>Toluene</td>
<td>1644</td>
<td>1644</td>
</tr>
<tr>
<td>Benzene</td>
<td>39212</td>
<td>39212</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1947</td>
<td>1947</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Design Data:</th>
<th>Density of Fluid (lb/cuft): 48.41</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Brake Power (hp): 0.31</td>
</tr>
<tr>
<td></td>
<td>Pump Head (ft): 5.95</td>
</tr>
<tr>
<td></td>
<td>Electricity Requirements (kW): 0.23</td>
</tr>
<tr>
<td></td>
<td>Material of Construction: Carbon Steel</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost, C_P, C_TDC</th>
<th>$5,100</th>
<th>$34,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## Section VI: Specification Sheets

### Distillation Column

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>DC-500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>500</td>
</tr>
<tr>
<td>No. Req'd</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

### Function
Separates "light" hydrocarbons from "heavy" hydrocarbons.

### Operation
Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th>Material</th>
<th>Feed: S-504</th>
<th>S-505</th>
<th>S-512</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>358214</td>
<td>143285</td>
<td>214929</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>177</td>
<td>236</td>
<td>209</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>60901</td>
<td>56067</td>
<td>4834</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>3670</td>
<td>3543</td>
<td>121</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5902</td>
<td>5484</td>
<td>418</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2613</td>
<td>0</td>
<td>2613</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16082</td>
<td>0</td>
<td>16082</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>28033</td>
<td>0</td>
<td>28033</td>
</tr>
<tr>
<td>Water</td>
<td>1709</td>
<td>0</td>
<td>1709</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>1003</td>
<td>890</td>
<td>113</td>
</tr>
<tr>
<td>Toluene</td>
<td>151529</td>
<td>6745</td>
<td>144784</td>
</tr>
<tr>
<td>Benzene</td>
<td>2557</td>
<td>0</td>
<td>2557</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>20320</td>
<td>20320</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20266</td>
<td>20254</td>
<td>12</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>30280</td>
<td>29376</td>
<td>304</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>6724</td>
<td>0</td>
<td>6724</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>0</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1331</td>
<td>0</td>
<td>1331</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>3463</td>
<td>0</td>
<td>3463</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>844</td>
<td>0</td>
<td>844</td>
</tr>
</tbody>
</table>

### Design Data:
- Stages: 30
- Feed Stage: 12
- Reflux Ratio: 0.86
- Height (ft): 68
- Diameter (ft): 16.5
- Material of Construction: Carbon Steel

### Cost, C_P, C_TDC
- $981,500
- $1,940,800

### Utilities:
- Electricity
- Steam

### Comments:
<table>
<thead>
<tr>
<th>Associated Component</th>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Tower</strong></td>
<td>Tray Type</td>
<td>Sieve</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
<td>14.7</td>
<td>psig</td>
</tr>
<tr>
<td></td>
<td>Bare Mod. Cost</td>
<td>$1,050,200</td>
<td></td>
</tr>
<tr>
<td><strong>Condenser</strong></td>
<td>Heat Duty</td>
<td>-30,638,080</td>
<td>BTU/hr</td>
</tr>
<tr>
<td></td>
<td>Area</td>
<td>1633</td>
<td>ft²</td>
</tr>
<tr>
<td></td>
<td>Shell Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Tube Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Tube Length</td>
<td>20</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td>Bare Mod. Cost</td>
<td>$115,600</td>
<td></td>
</tr>
<tr>
<td><strong>Reboiler</strong></td>
<td>Heat Duty</td>
<td>75,402,272</td>
<td>BTU/hr</td>
</tr>
<tr>
<td></td>
<td>Area</td>
<td>18984.3</td>
<td>ft²</td>
</tr>
<tr>
<td></td>
<td>Shell Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Tube Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bare Mod. Cost</td>
<td>$558,700</td>
<td></td>
</tr>
<tr>
<td><strong>Reflux Accumulator</strong></td>
<td>Liquid Volume</td>
<td>3022</td>
<td>gal</td>
</tr>
<tr>
<td></td>
<td>Height</td>
<td>17</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td>Diameter</td>
<td>5.5</td>
<td>ft</td>
</tr>
<tr>
<td></td>
<td>Bare Mod. Cost</td>
<td>$158,500</td>
<td></td>
</tr>
<tr>
<td><strong>Reflux Pump</strong></td>
<td>Bare Mod. Cost</td>
<td>$57,800</td>
<td></td>
</tr>
</tbody>
</table>
### Distillation Column

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: DC-501</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>501</td>
</tr>
<tr>
<td>No. Req’d</td>
<td>1</td>
</tr>
</tbody>
</table>

#### Function
- Separates heavy hydrocarbons from xylenes and similar compounds

#### Operation
- Continuous

#### Materials Handled:

<table>
<thead>
<tr>
<th>Feed: S-506</th>
<th>S-507</th>
<th>S-511</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>143285</td>
<td>143285</td>
</tr>
<tr>
<td>Temperature (F)</td>
<td>296</td>
<td>276</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>56067</td>
<td>5336</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>3549</td>
<td>2490</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5484</td>
<td>5216</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>830</td>
<td>877</td>
</tr>
<tr>
<td>Toluene</td>
<td>6745</td>
<td>6745</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>20320</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>20254</td>
<td>59.7</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>23976</td>
<td>5104</td>
</tr>
</tbody>
</table>

#### Design Data:
- Stages: 43
- Feed Stage: 16
- Reflux Ratio: 3
- Height (ft): 94
- Diameter (ft): 12.5
- Material of Construction: Carbon Steel

<table>
<thead>
<tr>
<th>Cost, CPE, CTEC</th>
<th>$775,000</th>
<th>$1,031,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td>Steam</td>
</tr>
</tbody>
</table>

#### Comments:

### Associated Component

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tower</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tray Type</td>
<td>Sieve</td>
<td></td>
</tr>
<tr>
<td>Pressure</td>
<td>1.7</td>
<td>psig</td>
</tr>
<tr>
<td>Bare Mod. Cost</td>
<td>$896,600</td>
<td></td>
</tr>
<tr>
<td>Condenser</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat Duty</td>
<td>-44,015,182</td>
<td>BTU/hr</td>
</tr>
<tr>
<td>Area</td>
<td>1585</td>
<td>ft²</td>
</tr>
<tr>
<td>Shell Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Tube Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Tube Length</td>
<td>20</td>
<td>ft</td>
</tr>
<tr>
<td>Bare Mod. Cost</td>
<td>$113,300</td>
<td></td>
</tr>
<tr>
<td>Reboiler</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat Duty</td>
<td>44,513,177</td>
<td>BTU/hr</td>
</tr>
<tr>
<td>Area</td>
<td>11493.4</td>
<td>ft²</td>
</tr>
<tr>
<td>Shell Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Tube Material</td>
<td>Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Bare Mod. Cost</td>
<td>$371,500</td>
<td></td>
</tr>
<tr>
<td>Reflux Accumulator</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Volume</td>
<td>5089</td>
<td>cal</td>
</tr>
<tr>
<td>Height</td>
<td>20.5</td>
<td>ft</td>
</tr>
<tr>
<td>Diameter</td>
<td>6.5</td>
<td>ft</td>
</tr>
<tr>
<td>Bare Mod. Cost</td>
<td>$160,600</td>
<td></td>
</tr>
<tr>
<td>Reflux Pump</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bare Mod. Cost</td>
<td>$67,200</td>
<td></td>
</tr>
</tbody>
</table>
### Distillation Column

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>Item No:</th>
<th>502</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. Req'd</td>
<td></td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

#### Function
Separates “light” hydrocarbons from “heavy” hydrocarbons.

#### Operation
Continuous

#### Materials Handled:

<table>
<thead>
<tr>
<th>Feed: 5-524</th>
<th>5-515</th>
<th>3-510</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>23,476</td>
<td>6,198</td>
</tr>
<tr>
<td>Temperature (F)</td>
<td>177</td>
<td>142</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>19374</td>
<td></td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2909</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5317</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2614</td>
<td>2614</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>1,102</td>
<td>1,102</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>582</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>14,431</td>
<td>1644</td>
</tr>
<tr>
<td>Benene</td>
<td>3,937</td>
<td>3,212</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1,947</td>
<td>1,947</td>
</tr>
</tbody>
</table>

#### Design Data:

- Stages: 20
- Feed Stage: 15
- Reflux Ratio: 12
- Height (ft): 48
- Diameter (ft): 22.5
- Material of Construction: Carbon Steel

#### Cost, CFB, CFD:

<table>
<thead>
<tr>
<th>Electricity</th>
<th>Steam</th>
</tr>
</thead>
<tbody>
<tr>
<td>$81,500</td>
<td>$2,485,600</td>
</tr>
</tbody>
</table>

#### Utilities:

- Electricity: $81,500
- Steam: $2,485,600

#### Comments:

#### Associated Component

<table>
<thead>
<tr>
<th>Tower</th>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Tray Type</td>
<td>Sieve</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
<td>14.7</td>
<td>psig</td>
</tr>
<tr>
<td></td>
<td>BareMod. Cost</td>
<td>$1,279,600</td>
<td></td>
</tr>
</tbody>
</table>

| Condenser | HeatDuty | -133,428,362 BTU/hr |
|           | Area      | 13,760 ft²           |
|           | ShellMaterial | Carbon Steel       |
|           | TubeMaterial  | Carbon Steel       |
|           | TubeLength   | 20 ft                |
|           | BareMod. Cost | $380,300          |

| Reboiler | HeatDuty | 146,774,702 BTU/hr |
|          | Area      | 15,246.5 ft²       |
|          | ShellMaterial | Carbon Steel       |
|          | TubeMaterial  | Carbon Steel       |
|          | BareMod. Cost | $522,000         |

| Reflux Accumulator | Liquid Volume | 13,326 gal |
|                   | Height       | 28 ft      |
|                   | Diameter     | 9 ft       |
|                   | BareMod. Cost | $193,500  |

| Reflux Pump | BareMod. Cost | $104,200 |
## Distillation Column

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: DC-503</th>
<th>Item No: 503</th>
<th>No. Req’d: 1</th>
</tr>
</thead>
</table>

### Function
Separates Toluene from other hydrocarbons for transalkylation.

### Operation
Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th>Feed: S-517</th>
<th>S-519</th>
<th>S-518</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>6186</td>
<td>39480</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>63</td>
<td>176</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2614</td>
<td>3</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16182</td>
<td>202</td>
</tr>
<tr>
<td>Toluene</td>
<td>1644</td>
<td>1644</td>
</tr>
<tr>
<td>Benzene</td>
<td>39212</td>
<td>37539</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1547</td>
<td>31</td>
</tr>
</tbody>
</table>

### Design Data:
- Stages: 17
- Feed Stage: 145
- Reflux Ratio: 3
- Height (ft): 42
- Diameter (ft): 7
- Material of Construction: Carbon Steel

### Cost, C_{FR}, C_{MB}:
- Cost: $438,200
- $1,010,900

### Utilities:
- Electricity
- Steam

### Comments:

#### Associated Component

**Tower**
- Tray: Sieve
- Pressure: 14.7 psig
- Bare Mod. Cost: $330,800

**Condenser**
- Heat Duty: -11,086,679 BTU/hr
- Area: 18423 ft²
- Shell Material: Carbon Steel
- Tube Material: Carbon Steel
- Tube Length: 20 ft
- Bare Mod. Cost: $421,600

**Reboiler**
- Heat Duty: 16,543,353 BTU/hr
- Area: 938 ft²
- Shell Material: Carbon Steel
- Tube Material: Carbon Steel
- Bare Mod. Cost: $113,500

**Reflux Accumulator**
- Liquid Volume: 1128 gal
- Height: 12 ft
- Diameter: 4 ft
- Bare Mod. Cost: $106,000

**Reflux Pump**
- Bare Mod. Cost: $39,000
## Heat Exchanger

### Identification
- **Item:** HX-500
- **Item No.:** 500
- **No. Req'd:** 1

### Function
- Cools the xylene other aromatic mix before the crystallizer.

### Operation
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th><strong>Shell Side</strong></th>
<th></th>
<th><strong>Tube Side</strong></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stream In:</td>
<td>Stream Out:</td>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td></td>
<td>S-521</td>
<td>S-508</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>74508</td>
<td>74508</td>
<td>74508</td>
<td>74508</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>60</td>
<td>-22</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td>53336</td>
<td>53336</td>
<td>2490</td>
<td>2490</td>
</tr>
<tr>
<td>p-Xylene</td>
<td></td>
<td></td>
<td>5216</td>
<td>5216</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2490</td>
<td></td>
<td>877</td>
<td>877</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5216</td>
<td></td>
<td>6745</td>
<td>6745</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>877</td>
<td></td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Toluene</td>
<td>6745</td>
<td></td>
<td>5184</td>
<td>5184</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>60</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>5184</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Design Data:
- **Heat Duty (BTU):** -2,163,272
- **Overall Heat Coefficient (BTU/hr-ft^2°C):** 50
- **Heat Transfer Area (ft^2):** 2858
- **Type:** Floating Head
- **Material of Construction:** Shell: Carbon Steel, Tube: Carbon Steel

### Cost, C_{PB}, C_{TDC}:
- **$54,200**
- **$150,200**

### Utilities:

### Comments:
- Heat from furnace
# Section VI: Specification Sheets

## Heat Exchanger

### Identification
- Item: HX-501
- Item No: 501
- No. Req'd: 1

### Function
Cools the xylene other aromatic mix before the crystallizer.

### Operation
Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>74508</td>
<td>74508</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>226</td>
<td>60</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>53336</td>
<td>53336</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2490</td>
<td>2490</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5216</td>
<td>5216</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>877</td>
<td>877</td>
</tr>
<tr>
<td>Toluene</td>
<td>6745</td>
<td>6745</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>5184</td>
<td>5184</td>
</tr>
</tbody>
</table>

### Design Data:
- Heat Duty (BTU): 5,221,359
- Overall Heat Coefficient (BTU/hr-ft²): 80
- Heat Transfer Area (ft²): 907
- Type: Floating Head
- Material of Construction:
  - Shell: Carbon Steel
  - Tube: Carbon Steel

### Cost, \(C_{PB}, C_{TDC}\):
- \(C_{PB}\): $24,200
- \(C_{TDC}\): $96,300

### Utilities:

### Comments:
Heat from furnace
# Separator

**Identification**
- Item: SEP-500
- Item No: 500
- No. Req’d: 1

**Function**
- 3 phase separator

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Streams In:</th>
<th></th>
<th>Streams Out:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-508</td>
<td>S-510</td>
<td>S-509</td>
<td></td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>67763</td>
<td>50431</td>
<td>17332</td>
<td></td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>-22</td>
<td>-22</td>
<td>-22</td>
<td></td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>53336</td>
<td></td>
<td>3505</td>
<td></td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2490</td>
<td>0</td>
<td>2490</td>
<td></td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5216</td>
<td>0</td>
<td>5216</td>
<td></td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>877</td>
<td>0</td>
<td>877</td>
<td></td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>60</td>
<td>0</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>5184</td>
<td>0</td>
<td>5184</td>
<td></td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU/hr): -85
- Height (ft): 16.5
- Diameter (ft): 7.5
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}:**
- $15,000,000
- $15,000,000

**Utilities:**

**Comments:** See utilities section
## Pump

**Identification**
- Item: P-601
- Item No: 601
- No. Req’d: 1

**Function**
To pump the sorbitol water stream from HX-601 to MIX-502.

**Operation**
Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th>Materials</th>
<th>Feed: S-603</th>
<th>Exit: S-604</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>85780</td>
<td>85780</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>182</td>
<td>182</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>19973</td>
<td>19973</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2909</td>
<td>2909</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5817</td>
<td>5817</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2613</td>
<td>2613</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16082</td>
<td>16082</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>582</td>
<td>582</td>
</tr>
<tr>
<td>Toluene</td>
<td>14350</td>
<td>14350</td>
</tr>
<tr>
<td>Benzene</td>
<td>21137</td>
<td>21137</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1931</td>
<td>1931</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/ft³): 48.5
- Brake Power (hp): 0.89
- Pump Head (ft): 5.9
- Electricity Requirements (kW): 0.67
- Material of Construction: Carbon Steel

**Cost, C_{PB}, C_{TDC}**
- $7,900
- $54,200

**Utilities:**
- Electricity

**Comments:**
## Heat Exchanger

### Identification
- Item: HX-600
- Item No: 600
- No. Req'd: 1

### Function Operation
- Converts the distillate of DC-500 to transalkylation reactor temperature.
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th>Shell Side</th>
<th>Stream In</th>
<th>Stream Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>214922</td>
<td>214922</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>209</td>
<td>850</td>
</tr>
</tbody>
</table>

#### Composition (lb/hr)
- **p-Xylene**: 4834
- **o-Xylene**: 120
- **m-Xylene**: 417
- **n-Butane**: 2613
- **n-Pentane**: 16082
- **n-Hexane**: 28033
- **Water**: 1709
- **Hydrogen**: 0.7
- **Ethylbenzene**: 113
- **Toluene**: 144780
- **Benzene**: 2557
- **Naphthalene**: 0.3
- **1,2,4-Trimethylbenzene**: 12
- **Isopropylbenzene**: 304
- **n-Heptane**: 6723
- **1-Butene**: 386
- **1-Pentene**: 1931
- **1-Hexene**: 3463
- **1-Heptene**: 844

### Design Data:
- Heat Duty (BTU): 527,756,123
- Overall Heat Coefficient (BTU/h): 50
- Heat Transfer Area (ft²): ??
- Type: Floating Head
- Material of Construction:
  - Shell: Carbon Steel
  - Tube: Carbon Steel

### Cost, C_{PB}, C_{TDC}:
- $96,700
- $541,900

### Utilities:

### Comments:
- Heat from furnace
# Heat Exchanger

## Identification
- Item: HX-601
- Item No: 601
- No. Req'd: 1

## Function
- Cools the transalkylation reactor product with cooling water.
- Continuous

## Operation

<table>
<thead>
<tr>
<th>Materials Handled</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Stream In:</td>
<td>Stream Out:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td></td>
<td>568330</td>
</tr>
<tr>
<td>Temperature ('F)</td>
<td>90</td>
<td>120</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>19973</td>
<td>19973</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>2909</td>
<td>2909</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>5817</td>
<td>5817</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2613</td>
<td>2613</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16082</td>
<td>16082</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>582</td>
<td>582</td>
</tr>
<tr>
<td>Toluene</td>
<td>14350</td>
<td>14350</td>
</tr>
<tr>
<td>Benzene</td>
<td>21137</td>
<td>21137</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1931</td>
<td>1931</td>
</tr>
</tbody>
</table>

## Design Data
- Heat Duty (BTU): 18,586,806
- Overall Heat Coefficient (BTU/h): 80
- Heat Transfer Area (ft²): 1536
- Type: Floating Head
- Material of Construction
  - Shell: Carbon Steel
  - Tube: Carbon Steel

## Cost, C_{PB}, C_{TDC}:
- $34,800
- $119,400

## Utilities:
- Cooling Water

## Comments:
### Reactor

**Identification**
- Item: R-600
- Item No: 600
- No. Req'd: 1

**Function**
- Convert Sorbitol to Aromatics and other Hydrocarbons

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-600</td>
<td>S-601</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>214922</td>
<td>214922</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>850</td>
<td>850</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>4834</td>
<td>19971</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>120</td>
<td>2905</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>417</td>
<td>5814</td>
</tr>
<tr>
<td>n-Butane</td>
<td>2613</td>
<td>2613</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>16082</td>
<td>16080</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>28033</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>1709</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.7</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>113</td>
<td>582</td>
</tr>
<tr>
<td>Toluene</td>
<td>144780</td>
<td>143506</td>
</tr>
<tr>
<td>Benzene</td>
<td>2557</td>
<td>21134</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>0.3</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>12</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>304</td>
<td>0</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>6723</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>386</td>
<td>386</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>1931</td>
<td>1931</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>3463</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>844</td>
<td>0</td>
</tr>
</tbody>
</table>

**Design Data:**
- Volume (gal): 9254.01
- Working Vol initial (L): 24518
- Working Vol at end (L): 24518
- Height (ft): 28
- Diameter (ft): 7.5
- Material of Construction: Low Alloy Steel

**Cost, C_{PB}, C_{TDC}:**
- $310,900
- $567,800

**Utilities:**

**Comments:**
## Pump

### Identification
- **Item:** P-700
- **Item No:** 700
- **No. Req’d:** 2

### Function
- **Operation:** Pump Dowtherm A to HX-701
- **Materials Handled:** Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-713</th>
<th>Exit: S-721</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>2650000</td>
<td>2660000</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>698</td>
<td>698</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>2650000</td>
<td>2660000</td>
</tr>
<tr>
<td>Dowtherm A</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Design Data:
- **Density of Fluid (lb/cuft):** 45.29
- **Brake Power (hp):** 9.94
- **Pump Head (ft):** 79.13
- **Electricity Requirements (kW):** 7.84
- **Material of Construction:** 304 Stainless Steel

### Cost, \( C_{PB}, C_{TDC} \)
- **$51,300**
- **$481,700**

### Utilities:
- **Electricity**

### Comments:
<table>
<thead>
<tr>
<th><strong>Pump</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Function Operation</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
</tr>
<tr>
<td>Temperature (°F)</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
</tr>
<tr>
<td>Dowtherm A</td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Cost, C_P, C_TDC</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Comments:</strong></td>
</tr>
</tbody>
</table>
## Section VI: Specification Sheets

### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>P-703</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>703</td>
</tr>
<tr>
<td>No. Req'd</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

### Function

- Operation: Pumps molten salt to P-704.
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Feed: P-723</th>
<th>Exit: P-723-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>1176095</td>
<td>1176095</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>414</td>
<td>414</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molten Salt</td>
<td>1176095</td>
<td>1176095</td>
</tr>
</tbody>
</table>

### Design Data:

- Density of Fluid (lb/cuft): 62.07
- Brake Power (hp): 3.33
- Pump Head (ft): 163.8
- Electricity Requirements (kW): 60.98
- Material of Construction: 304 Stainless Steel

### Cost, $C_{PB}$, $C_{TDC}$

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost, $C_{PB}$, $C_{TDC}$</td>
<td>$27,100</td>
<td>$114,000</td>
</tr>
</tbody>
</table>

### Utilities:

- Electricity

### Comments:
<table>
<thead>
<tr>
<th><strong>Pump</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Function</strong></td>
</tr>
<tr>
<td><strong>Operation</strong></td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Cost, C_{PB}, C_{TDC}</strong></td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td>Identification</td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

| Function Operation | Pumps steam for HX-301. | Continuous |

<table>
<thead>
<tr>
<th>Materials Handled:</th>
<th>Feed: S-725</th>
<th>S-730</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>39600</td>
<td>39600</td>
</tr>
<tr>
<td>Temperature(°F)</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>39600</td>
<td>39600</td>
</tr>
<tr>
<td>Water</td>
<td>39600</td>
<td>39600</td>
</tr>
</tbody>
</table>

| Design Data: | Density of Fluid (lb/cuft): | 61.61 |
|             | Brake Power (hp):            | 0.14  |
|             | Pump Head (ft):              | 4.68  |
|             | Electricity Requirements (kW): | 0.18 |
|             | Material of Construction:    | Carbon Steel |

<p>| Cost, ( C_{PB} ), ( C_{TDC} ) | $4,500 | $35,400 |
| Utilities: | Electricity |
| Comments: |  |</p>
<table>
<thead>
<tr>
<th><strong>Pump</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td>Item:</td>
</tr>
<tr>
<td>Item No:</td>
</tr>
<tr>
<td>No. Req'd</td>
</tr>
<tr>
<td><strong>Function</strong></td>
</tr>
<tr>
<td><strong>Operation</strong></td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td><strong>Feed: S-725IN</strong></td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
</tr>
<tr>
<td>Temperature(°F)</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
</tr>
<tr>
<td>Water</td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td>Density of Fluid (lb/cuft):</td>
</tr>
<tr>
<td>Brake Power (hp):</td>
</tr>
<tr>
<td>Pump Head (ft):</td>
</tr>
<tr>
<td>Electricity Requirements (kW):</td>
</tr>
<tr>
<td>Material of Construction:</td>
</tr>
<tr>
<td><strong>Cost, ( C_{PB}, C_{TDC} )</strong></td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td><strong>Comments:</strong></td>
</tr>
</tbody>
</table>
## Section VI: Specification Sheets

<table>
<thead>
<tr>
<th><strong>Pump</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Function</strong></td>
</tr>
<tr>
<td><strong>Operation</strong></td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td><strong>Cost, $C_{PB}, C_{TDC}$</strong></td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td><strong>Comments:</strong></td>
</tr>
<tr>
<td>Identification</td>
</tr>
<tr>
<td>----------------------</td>
</tr>
<tr>
<td>Item No:</td>
</tr>
<tr>
<td>No. Req'd</td>
</tr>
</tbody>
</table>

| Function Operation   | Pumps steam for HX-301. | Continuous |

<table>
<thead>
<tr>
<th>Materials Handled:</th>
<th>Feed: S-726IN</th>
<th>S-731IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>86174</td>
<td>86174</td>
</tr>
<tr>
<td>Temperature(°F)</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Water</td>
<td>86174</td>
</tr>
<tr>
<td></td>
<td></td>
<td>86174</td>
</tr>
</tbody>
</table>

| Design Data:         | Density of Fluid (lb/cuft): 61.61 |
|----------------------| Brake Power (hp): 0.51 |
|                      | Pump Head (ft): 7.02 |
|                      | Electricity Requirements (kW): 0.38 |
|                      | Material of Construction: Carbon Steel |

| Cost, C_{PB}, C_{TDC}| $4,500 | $36,600 |

<table>
<thead>
<tr>
<th>Utilities:</th>
<th>Electricity</th>
</tr>
</thead>
</table>

| Comments:            |             |
## Section VI: Specification Sheets

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item:</th>
<th>P-707</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td></td>
<td>707</td>
</tr>
<tr>
<td>No. Req'd</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

### Function Operation

- Pumps steam for RB-501.
- Continuous

### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-727</th>
<th>S-732</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>53087</td>
<td>53087</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>53087</td>
<td>53087</td>
</tr>
</tbody>
</table>

### Design Data:

- Density of Fluid (lb/cuft): 61.61
- Brake Power (hp): 0.23
- Pump Head (ft): 4.68
- Electricity Requirements (kW): 0.17
- Material of Construction: Carbon Steel

### Cost, $C_{PB}$, $C_{TDC}$

- $C_{PB}$: 4,700
- $C_{TDC}$: 36,600

### Utilities:

- Electricity

### Comments:
<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-708</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>708</td>
</tr>
<tr>
<td>No. Req’d</td>
<td>1</td>
</tr>
</tbody>
</table>

| Function          | Pumps steam for RB-502. |
| Operation         | Continuous            |

| Materials Handled: | Feed: S-728 | S-733 |
|--------------------|-------------|
| Quantity (lb/hr)   | 159192      |
| Temperature(°F)    | 90          |
| Composition (lb/hr)|            |
| Water              | 159192      |

| Design Data:       | Density of Fluid (lb/cuft): 61.61 |
|                    | Brake Power (hp): 0.56          |
|                    | Pump Head (ft): 4.68            |
|                    | Electricity Requirements (kW): 0.47 |
|                    | Material of Construction: Carbon Steel |

<table>
<thead>
<tr>
<th>Cost, $C_{PB}, C_{TC}$</th>
<th>$6,300$</th>
<th>$43,900$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-708IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Item No:</td>
<td>708IN</td>
</tr>
<tr>
<td>No. Req'd</td>
<td>1</td>
</tr>
</tbody>
</table>

| Function Operation     | Pumps steam for RB-502. Continuous |

#### Materials Handled:

<table>
<thead>
<tr>
<th></th>
<th>Feed: S-728IN</th>
<th>S-733IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>159192</td>
<td>159192</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>159192</td>
<td>159192</td>
</tr>
</tbody>
</table>

#### Design Data:

- Density of Fluid (lb/cuft): 61.61
- Brake Power (hp): 0.84
- Pump Head (ft): 7.02
- Electricity Requirements (kW): 0.63
- Material of Construction: Carbon Steel

<table>
<thead>
<tr>
<th>Cost, (C_{PB}, C_{TDC})</th>
<th>$6,300</th>
<th>$43,900</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Identification</td>
<td>Item: P-709</td>
<td>Item No: 709</td>
</tr>
<tr>
<td>Function</td>
<td>Pumps steam for RB-503.</td>
<td></td>
</tr>
<tr>
<td>Operation</td>
<td>Continuous</td>
<td></td>
</tr>
<tr>
<td>Materials Handled:</td>
<td>Feed: S-729</td>
<td>S-734</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>17143</td>
<td>17143</td>
</tr>
<tr>
<td>Temperature(°F)</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>Water 17143</td>
<td>Water 17143</td>
</tr>
<tr>
<td>Design Data:</td>
<td>Density of Fluid (lb/cuft): 61.61</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Brake Power (hp): 0.11</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pump Head (ft): 4.68</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Electricity Requirements (kW): 0.08</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Material of Construction: Carbon Steel</td>
<td></td>
</tr>
<tr>
<td>Cost, $C_{PB}$, $C_{TDC}$</td>
<td>$4,300$</td>
<td>$31,600$</td>
</tr>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Section VI: Specification Sheets

#### Pump

<table>
<thead>
<tr>
<th>Identification</th>
<th>Item: P-709IN</th>
<th>Item No: 709IN</th>
<th>No. Req'd: 1</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Function</th>
<th>Pumps steam for RB-503.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operation</td>
<td>Continuous</td>
</tr>
</tbody>
</table>

#### Materials Handled:

<table>
<thead>
<tr>
<th>Feed: S-729IN</th>
<th>S-734IN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>17143</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td>17143</td>
</tr>
<tr>
<td>Water</td>
<td>17143</td>
</tr>
</tbody>
</table>

#### Design Data:

- Density of Fluid (lb/cuft): 61.61
- Brake Power (hp): 0.16
- Pump Head (ft): 7.02
- Electricity Requirements (kW): 0.12
- Material of Construction: Carbon Steel

<table>
<thead>
<tr>
<th>Cost, $C_{PB}, C_{TDC}$</th>
<th>$4,300$</th>
<th>$31,600$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities:</td>
<td>Electricity</td>
<td></td>
</tr>
<tr>
<td>Comments:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Identification</td>
<td>Item: ST-700</td>
<td></td>
</tr>
<tr>
<td>----------------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>Item No:</td>
<td>700</td>
<td></td>
</tr>
<tr>
<td>No. Req'd</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Function</th>
<th>Store Dowtherm A briefly.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operation</td>
<td>Continuous</td>
</tr>
</tbody>
</table>

| Materials Handled: |

<table>
<thead>
<tr>
<th>Feed: Dowtherm A</th>
<th>Exit: Dowtherm A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>5320000</td>
</tr>
<tr>
<td>Temperature(°F)</td>
<td>698</td>
</tr>
<tr>
<td>Composition (lb/hr) Dowtherm A</td>
<td>5320000</td>
</tr>
</tbody>
</table>

| Design Data: |
| Density of Fluid (lb/cuft): | 45.29 |
| Volume (gal): | 124,000 |
| Pressure (psia) | 93.69 |
| Capacity Usage | 70% |
| Material of Construction: | Low Alloy Steel |

<table>
<thead>
<tr>
<th>Cost, $</th>
<th>C&lt;sub&gt;PB&lt;/sub&gt;, $</th>
<th>C&lt;sub&gt;TDC&lt;/sub&gt;, $</th>
</tr>
</thead>
<tbody>
<tr>
<td>$599,900</td>
<td>$719,900</td>
<td></td>
</tr>
</tbody>
</table>

Utilities: 
Comments:
### Storage Tank

**Identification**
- Item: ST-701
- Item No: 701
- No. Req’d: 1

**Function**
- Store Dowtherm A briefly.

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Feed: Solar Salt</th>
<th>Exit: Solar Salt</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity (lb/hr)</td>
<td>117,609.5</td>
<td>117,609.5</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>900</td>
<td>900</td>
</tr>
<tr>
<td>Composition (lb/hr) Dowtherm A</td>
<td>117,609.5</td>
<td>117,609.5</td>
</tr>
</tbody>
</table>

**Design Data:**
- Density of Fluid (lb/cuft): 62.07
- Volume (gal): 639,300
- Pressure (psia): 17.7
- Capacity Usage: 70%
- Material of Construction: 304 Stainless Steel

**Cost, $P_B, C_{TDC}**
- $329,400
- $658,800

**Utilities:**

**Comments:**
<table>
<thead>
<tr>
<th><strong>Heat Exchanger</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Identification</strong></td>
</tr>
<tr>
<td>Item:</td>
</tr>
<tr>
<td>Item No: 703</td>
</tr>
<tr>
<td>No. Req’d 2</td>
</tr>
<tr>
<td><strong>Function</strong></td>
</tr>
<tr>
<td>Condenses Dowtherm A</td>
</tr>
<tr>
<td>Operation</td>
</tr>
<tr>
<td>Continuous</td>
</tr>
<tr>
<td><strong>Materials Handled:</strong></td>
</tr>
<tr>
<td><strong>Shell Side</strong></td>
</tr>
<tr>
<td>Stream In: S-715</td>
</tr>
<tr>
<td>Stream Out: S-717</td>
</tr>
<tr>
<td><strong>Tube Side</strong></td>
</tr>
<tr>
<td>Stream In:</td>
</tr>
<tr>
<td>Stream Out:</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
</tr>
<tr>
<td>Temperature(°F)</td>
</tr>
<tr>
<td><strong>Dowtherm A</strong></td>
</tr>
<tr>
<td>Dental: 266000</td>
</tr>
<tr>
<td>Dental: 266000</td>
</tr>
<tr>
<td><strong>Design Data:</strong></td>
</tr>
<tr>
<td>Heat Duty (BTU):</td>
</tr>
<tr>
<td>Overall Heat Coefficient (BTU/hr-ft²°F)</td>
</tr>
<tr>
<td>Heat Transfer Area (ft²):</td>
</tr>
<tr>
<td>Type: Floating Head</td>
</tr>
<tr>
<td>Material of Construction</td>
</tr>
<tr>
<td>Shell: 304 Stainless Steel</td>
</tr>
<tr>
<td>Tube: 304 Stainless Steel</td>
</tr>
<tr>
<td><strong>Cost, C_PB, C_TDC:</strong></td>
</tr>
<tr>
<td>$42,700</td>
</tr>
<tr>
<td>$197,800</td>
</tr>
<tr>
<td><strong>Utilities:</strong></td>
</tr>
<tr>
<td><strong>Comments:</strong></td>
</tr>
</tbody>
</table>
### Section VI: Specification Sheets

#### Furnace

**Identification**
- Item: FRN-701
- Item No: 701
- No. Req'd: 2

**Function**
- Operation: Dowtherm A heater
- Materials Handled: Continuous

<table>
<thead>
<tr>
<th></th>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-703</td>
<td>S-707</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>89889</td>
<td>3750111</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90</td>
<td>256</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>1951</td>
<td>0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>1132</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>1754</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>8966</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>1941</td>
<td>0</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>7410</td>
<td>0</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>1433</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>29809</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>8122</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>124</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>870026</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>2880085</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>285</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>2241</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>577</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>6471</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>6467</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>9610</td>
<td>0</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>125</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>312</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>935</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>206</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>18</td>
<td>0</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU/hr): -263,915,627
- Height (ft): 13
- Diameter (ft): 3
- Material of Construction: Carbon Steel

**Cost, C_{FB}, C_{TDC}:**
- $5,186,600
- $5,186,000

**Utilities:**

**Comments:**
Furnace

**Identification**
- Item: FRN-700
- Item No: 700
- No. Req'd: 1

**Function**
- Molten Salt heater

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Streams In:</th>
<th>Streams Out:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-701</td>
<td>S-705</td>
</tr>
<tr>
<td><strong>Quantity (lb/hr)</strong></td>
<td>22916</td>
<td>750022</td>
</tr>
<tr>
<td><strong>Temperature (°F)</strong></td>
<td>90</td>
<td>256</td>
</tr>
<tr>
<td><strong>Composition (lb/hr)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>497</td>
<td>0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>289</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>445</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>2286</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>495</td>
<td>0</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>1890</td>
<td>0</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>365</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>7600</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>2071</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>32</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>174005</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>576017</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>73</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>571</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>147</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>1650</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>1650</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>2450</td>
<td>0</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>32</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>79</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>238</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>52</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>4</td>
<td>0</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU/hr): -71,354,717
- Height (ft): 9.5
- Diameter (ft): 2
- Material of Construction: 304 Stainless Steel

**Cost, C_{PB}, C_{TDC}**
- $1,626,600
- $3,253,200

**Utilities:**

**Comments:**
### Section VI: Specification Sheets

#### Furnace

**Identification**
- Item: FRN-703
- Item No: 703
- No. Req'd: 1

**Function**
- Provides steam for reboilers, WC-500 and HX-301

**Operation**
- Continuous

**Materials Handled:**

<table>
<thead>
<tr>
<th></th>
<th>Streams In</th>
<th>Streams Out</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S-704</td>
<td>S-711</td>
</tr>
<tr>
<td>Quantity (lb/hr)</td>
<td>79783</td>
<td>8365631</td>
</tr>
<tr>
<td>Temperature (°F)</td>
<td>90</td>
<td>256</td>
</tr>
<tr>
<td>Composition (lb/hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>1732</td>
<td>0</td>
</tr>
<tr>
<td>o-Xylene</td>
<td>1005</td>
<td>0</td>
</tr>
<tr>
<td>m-Xylene</td>
<td>1550</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>7959</td>
<td>0</td>
</tr>
<tr>
<td>n-Butane</td>
<td>1723</td>
<td>0</td>
</tr>
<tr>
<td>n-Pentane</td>
<td>6577</td>
<td>0</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>1272</td>
<td>0</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>26460</td>
<td>0</td>
</tr>
<tr>
<td>Water</td>
<td>7210</td>
<td>0</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>110</td>
<td>0</td>
</tr>
<tr>
<td>Oxygen</td>
<td>0</td>
<td>1940826</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0</td>
<td>6424805</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>253</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>1989</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>512</td>
<td>0</td>
</tr>
<tr>
<td>Naphthalene</td>
<td>5744</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>5740</td>
<td>0</td>
</tr>
<tr>
<td>Isopropylbenzene</td>
<td>8530</td>
<td>0</td>
</tr>
<tr>
<td>n-Heptane</td>
<td>111</td>
<td>0</td>
</tr>
<tr>
<td>1-Butene</td>
<td>277</td>
<td>0</td>
</tr>
<tr>
<td>1-Pentene</td>
<td>830</td>
<td>0</td>
</tr>
<tr>
<td>1-Hexene</td>
<td>183</td>
<td>0</td>
</tr>
<tr>
<td>1-Heptene</td>
<td>16</td>
<td>0</td>
</tr>
</tbody>
</table>

**Design Data:**
- Heat Duty (BTU/hr): -315,781,138
- Height (ft): 12.5
- Diameter (ft): 3
- Material of Construction: Carbon Steel

**Cost, C_{PB}, C_{TDC}:**
- $1,495,600

**Utilities:**

**Comments:**
Section VII
Other Considerations
VII. OTHER CONSIDERATIONS

Alternate Design Considerations

Removal of Aqueous Phase Reforming Section
A major section of this process is based upon Virent Corporation’s aqueous phase reforming technology, which is detailed in WO2007/075476-A2 and several other patents. The appeal of the aqueous phase reforming technology is that it generates hydrogen in situ for use in hydrogenation, a necessary step in getting from oxygenated hydrocarbon to p-xylene. Unfortunately, however, the analysis presented herein reveals that APR is quite costly due to the compression needs and exotic catalysts. This resulted in consideration of removing the APR section. Doing so would eliminate about six process units, $2M in electricity, and over $78M of catalyst technology. The substitute cost would be the external purchase of hydrogen. However, purchasing hydrogen from an economical source goes hand-in-hand with purchasing it from a non-green source, which goes against the purpose of this design. This would not be justified unless savings and impact on NPV were dramatic. As it turns out, even removing the entire 300 section of the flowsheet has limited impact on bottom line profitability. Although the large capital outlay, much of which is directly traceable to section 300, contributes to a large negative NPV, the major cost driver is input materials. Therefore, even a change as substantial as this is not enough to turn NPV positive (although it should be noted that IRR becomes positive, without accounting for the cost of hydrogen). Thus, this design is discarded because its benefit is not nearly enough to justify its lack of sustainability.

Woody Biomass with Three-Phase Hot Water Extraction
Due to its high per pound cost, corn dry grind was never an attractive feedstock. Of the two remaining options, woody biomass was the cheaper raw material. However, two unique processing steps were necessary to convert it into usable simple sugars: extraction of the cellulose, and
enzymatic cleaving of the ether bonds in the cellulose chains. In contrast, molasses was slightly more expensive upfront, but required only the additional clarification step prior to hydrolysis.

Initially, separating the biomass into its different components, each of which served a different purpose, posed a challenge. However, US Patent 5730837 described a unique, one-step sequence that generated three phases, each of which contained one of the necessary components. In short, the biomass would be heated in a mixture of ketone and water insoluble at room temperature until a single-phase solution was obtained. Then, by cooling and/or adding additional water, the three phases would separate into three separate phases. The cellulose would remain as solid precipitate to filter out and convert enzymatically into simple sugars. The hemicelluloses and simple sugars would remain aqueous, and could be sent for completed breakdown into simple sugars. Finally, the lignin would remain in the organic solvent, most of which could be recovered before sending the lignin to the furnace to burn. An example of this process is shown in Figure 14 below.
Even with this streamlined separation process, the high cost of enzymes required to process the cellulose, from which the majority of the sugar for para-xylene production would be derived, rendered woody biomass economically inferior to molasses.

**Alternative Separation Scheme**

The separation scheme used for the renewable production of para-xylene can be varied drastically. An alternative design is presented in Figure 15 below. Note that the blocks are labeled such that the columns in the actual process have the same light and heavy key’s as blocks with the same name below (e.g. DC-500 always separates between xylenes and toluene).
In this scheme, DC-500 and DC-501 have been switched, meaning the heavy aromatics are taken off before the light in the isolation of para-xylene. While certainly possible, this option was not pursued because the separation between para-xylene and the next heaviest species, isopropylbenzene, in DC-501 is far more difficult and requires a larger column and more stages than the xylene/toluene separation in DC-500. It is cheaper to deal with the larger quantity of material in the shorter column, DC-500. In addition, because the three phase separator operates at cooler temperatures than the distillation columns, it is also cheaper to do the lower-temperature distillation (DC-500) first, rather than heating to the higher temperature and then cooling again.

In this scheme, DC-502 and DC-503 have also been switched. This decision can be made independently of the order of DC-500 and DC-501. In this case, the pentane separation is easier, and, all other things being equal, it would be cheaper to drive off the alkanes first, as depicted above. However, the transalkylation occurs at temperatures higher than the distillation columns. As such, it
Section VII: Other Considerations

is actually cheaper to take off the heavy constituents, xylene and toluene, as they condense, rather than to condense everything other than the alkanes and reheat afterwards, as depicted above.

**Invertase-Catalyzed Sucrose Hydrolysis**

In the food industry, the enzyme invertase is commonly used to catalyze the sucrose hydrolysis reaction. It is a proven technology which operates under easily attainable conditions. Invertase is added to a 60% sucrose solution and then heated to 60 °C. Citric acid is then added to make the solution have a pH of 4.5. The invertase takes 12 hours to fully convert the sucrose into fructose and glucose.

However, the prohibiting factor is that invertase costs around $40 per kilogram and a kilogram of invertase is required to invert one metric ton of sucrose. Invertase is also difficult to recover from the product. Because of the high cost, the choice was made to use a zeolite catalyst in a fixed bed reactor instead.

**Plant Startup**

Because the hydrogenation section requires a large amount of hydrogen (3655 lbmol per hour), a supply of hydrogen will have to be available until the plant can produce enough hydrogen to sustain itself through the aqueous phase reforming reaction. The pressure swing adsorption contains a large pressure vessel used to store up to a 21 hour supply of hydrogen. This storage vessel will be able to supply hydrogen for any future plant startups after the first time.

The furnaces are fired from byproduct gases such as alkanes and aromatics so a supply of natural gas will have to be available to fire the furnaces in order to produce process steam and heat the Dowtherm A and molten salt. Additionally, the salt will have to be melted if allowed to solidify.

On startup, auxiliary heat might have to be provided to several streams since streams farther down the process would not be heated to their expected values, causing heat exchangers to operate at
non-ideal conditions. Because the plant utilizes many heat exchangers to preheat and cool streams, this could pose a major challenge.

The aqueous phase separated from the flash vessel in the separation section (SEP-500) is used as cooling water for a high temperature stream, so a secondary source of cooling water must be provided to operate HX-601.

Sodium hydroxide is used as a catalyst in the APR reaction, and is recovered through the flash vessel after the reaction (F-300), so no additional sodium hydroxide needs to be added after startup. The sodium hydroxide will have to be added into the recycle loop as the plant starts up.

Environmental Considerations

The primary impact on the environment is the release of waste carbon dioxide. The plant releases approximately 1.5 million tons per year of carbon dioxide. In addition, 20,000 tons per year of carbon monoxide are released into the atmosphere. Approximately 10,000 tons per year of propane and other alkanes are released as well.

A 2005 report by the Center for Climate and Energy Solutions reported that the cost to sequester carbon dioxide ranged from $30 to $90 per ton of carbon dioxide. At $30 per ton it would cost $45 million per year to sequester all of the carbon released from the plant. This is clearly an expensive option, but it is not unfeasible given the expected $325M/yr revenue. That said, the operating margin is currently nowhere near able to support a variable cost of this magnitude.

The process also requires 40.3 bgal/y of water, or 11.8 bgal/y excluding HX-401. As noted earlier, HX-401 is a serious cause for concern, but it will likely be straightforward to discover improvements. Ignoring HX-401 for now, the process uses about 4.1 gal water/gal of p-xylene, which is higher than the industry benchmark of 3 gal/gal. However, it is close enough to be encouraging. In fact, excluding chilled water, the ratio is 3.7 gal/gal. Clearly there is room for
improvement in term of cooling water recycle. With a bit of careful consideration – specifically with regard to water cooling rates in open air – a zero-discharge plant is well within reach.

In addition, some organic compounds, mostly naphthalene, 1,2,4-trimethylbenzene, and isopropylbenzene, are encountered as waste products from DC-501. These compounds are currently burned in the furnace; however, they could be separated further and sold, although the economics of this have not been explored.

The plant succeeds at producing para-xylene from renewable sources. The only input to the process is molasses. Cooling water is used extensively, but the plant could easily switch to a closed loop cooling water system.

**Process Control**

The process operates at temperatures and pressures provided in specific examples found in patents and other relevant literature. Consequently, a narrow acceptable range of operating conditions are assumed for all sections of the process and all reactors in particular. Further research may reveal a wider range of acceptable operating conditions for some or all process units. However, the strategies for control explained within this section should still apply.

A full analysis of process control requirements, as well as the design of a corresponding system, falls beyond the scope of this report. However, the critical elements of the process variables to be controlled, as well as potential strategies for controlling these variables, are disclosed. Following the additional research recommended by this report, the following concerns should be addressed in the next iteration of this process’s design.

**Section 100: Hydrolysis**

The streams and blocks associated with hydrolysis must be controlled such that (a) the sucrose feed (S-100) to each hydrolysis reactor (R-100, R-101, and R-102) enters at 212.0 degrees
Castillo, Ernst, Lerch, Winchester
Fahrenheit and 41.1 psia, and (b) the glucose/fructose stream (S-119) is feed to hydrogenation at the proper pressure.

To set pressure, power to the pre-hydrolysis pumps (P-100, P-101, and P-102) and post-hydrolysis pumps (P-103, P-104, and P-105) will adjusted as necessary in response to readings from a pressure sensors, most likely variable capacitance differential pressure transducers.

The temperature poses a greater challenge, as it results only from the exchange of heat between the sucrose feeds (S-104, S-105, and S-106) and the condensation product streams (S-417, S-418, S-419). For mild temperature disturbances, increasing or decreasing the flow rate of the condensation product (S-416) would raise or lower (respectively) the temperature of the sucrose streams (S-106, S-107, and S-108) exiting the heat exchangers and entering the hydrolysis reactors. This control system would require holdup tanks both preceding and following the heat exchangers (HX-100, HX-101, and HX-102) in order to ensure no disturbances elsewhere in the process. Because cooling water is ultimately used to bring the condensation product to an appropriate temperature for separation, the flow rate of the cooling water can be varied to compensate for the discrepancies in cooling achieved in the heat exchangers (HX-100, HX-101, and HX-102) as a result of these techniques. If severe disturbances are expected, the process will require investment in an additional heater and/or cooler to which a fraction of the disturbed stream (S-100) can be diverted.

Section 200: Hydrogenation
Successful hydrogenation will rely on proper control of the temperature and pressure of both the hydrogen (S-316) and sugar (S-226) feeds to the reactors. Discussion of the hydrogen stream (S-316) can be found in this section under Aqueous Phase Reforming, below. Pressure of the sugar stream (S-119) was set using automated pumps (P-103, P-104, and P-105) discussed under Hydrolysis, above. Cooling water (CW-100) in heat exchanger (HX-200) sets the temperature. As such, the flow rate of the cooling water (CW-100) can be varied to achieve the desired temperature.
Section VII: Other Considerations

Section 300: Aqueous Phase Reforming

Although more complex than previous sections, the Aqueous Phase Reforming has only one block that requires precise control: the reforming reactor itself (R-300). The feed stream (S-305) must enter the reactor at the desired conditions, 360 degrees Fahrenheit and 725 psia. The pressure is achieved through a pair of pumps (P-302 and P-300), and power to the latter can be varied based on information from a sensor, most likely a variable capacitance differential pressure transducer on the second pump’s feed stream (S-303) in order to achieve the desired pressure. Although heat is recovered from the hydrogen product stream (S-311) in a heat exchanger located between the pumps (HX-300), the temperature of the sorbitol feed (S-305) is ultimately set by a second heat exchanger (HX-301) that uses steam (S-727) heated by the furnace as a heat source. As such, the temperature or the flow rate of the steam (S-727) can be varied based on a temperature sensor, most likely a thermocouple on the pressurized sorbitol stream (S-304), to achieve the desired temperature.

Other streams of direct consequence include the exiting hydrogen (S-316) for hydrogenation and exiting sorbitol (S-402) for condensation; the alkanes leaving the separator are simply sent to the furnace. After recovering some heat in a first pair of exchangers (HX-300 and HX-400) as well as cooling prior to entering the compressor (HX-303 prior to flash drum F-301 and compressor SEP-300), the outlet temperature of the hydrogen is ultimately set by a final heat exchanger (HX-302) which uses cooling water; as such, the flow rate of the cooling water can be varied to control the temperature based on information obtained from a temperature sensor, most likely a thermocouple on the post-heat-recovery stream (S-315). The sorbitol outlet (S-402) undergoes recovers some heat from the hydrogen (S-314 in heat exchanger HX-400) but will undergo much more processing in the condensation region of the process before it must be fed to the condensation reactors (R-400, R-401, R-402, and R-403).
Section 400: Condensation

For condensation, feed sorbitol stream (S-407) must enter at the proper conditions, 204 degrees Fahrenheit and 640 psia. Both the transalkylation product (S-601) and pre-crystallization xylenes (S-507), from which heat is recovered via heat exchangers (HX-402 and HX-403), are cooled later using either cooling water or chilled water, and can more easily be controlled in those later exchangers. The sorbitol feed (S-407) ultimately enters the condensation reactors (R-400, R-401, R-402, and R-403) at the exit temperature of the final heat exchanger (HX-404), which uses Dowtherm A as a hot stream. Since the Dowtherm’s only function is to transfer heat from the furnace to the condensation feed, the temperature or flow rate of the Dowtherm can be varied based on temperature data from the pre-exchanger (HX-404) sorbitol stream (S-405) collected via sensor, most likely a thermocouple. Heat recovery and cooling of the condensation product stream (S-416) is discussed in other sections.

Section 500: Separation

The separations section of the process requires little control. All separators operate at atmospheric pressure, and the transalkylation product (S-604) is cooled in Section 600. The only streams requiring control are the crystallization feed (S-520) and initial condensation product (S-423). The crystallization feed temperature is controlled by changing the flow rate of chilled water (CW-502) and ethylene refrigerant through the two pre-crystallization heat-exchangers (HX-501 and REF-500) based on temperature data obtained from a sensor, most likely a thermocouple on the pre-cooling stream (S-520). Similarly, after expansion to near atmospheric pressure, the proper temperature for the condensation product (S-423) is achieved by exchanging heat with cooling water (CW-400) in a pre-separation heat exchanger (HX-401). If the temperature of the post-heat-recovery stream (S-423) varies, either randomly or as a result of the control system described for Section 100, the flow rate of the cooling water can be varied to compensate based on information from a temperature sensor, most likely a thermocouple, on the pre-cooling stream (S-424). If the flow rate
were to vary as a result of the same control scheme, the holdup tank previously discussed in Section 100 would be used to prevent disturbance in Section 500.

Following the first three-phase separator (SEP-500), each distillation column (DC-500, DC-501, DC-502, and DC-503) is designed to operate with feed at the outlet temperature from the previous column. The designs are also robust enough that mild variation in the outlet temperatures does not dramatically affect the quality of separation. Properties of all streams exiting Section 500 are controlled elsewhere in the process: the vapor (S-500) from the three-phase separator (SEP-500), the heavy aromatics (S-509) from the crystallizer (SEP-501) and the alkanes (S-518) from the second post-transalkylation column (DC-503) are burned in the furnace; the distillate (S-512) from the first column (DC-500) is heated elsewhere prior to transalkylation; the xylenes-rich distillate (S-507) from the second column (DC-501) is cooled using heat recovery and chilled water prior to crystallization; finally, the benzene in the bottoms (S-519) from the second post-transalkylation column (DC-503) and para-xylene (S-510) leaving the crystallizer (SEP-501) are final products requiring no further treatment. Look at SC-500 for three-phase separation calculation.

Section 600: Transalkylation

The temperature and pressure of the transalkylation feed (S-600) must be controlled to the specified temperature and pressure, 850 degrees Fahrenheit and 150 psia. To achieve these conditions, the distillate (S-512) from the first distillation column (DC-500) is heated in a heat exchanger (HX-600) using molten-salt (S-723). Since the salt’s only function is to heat the transalkylation feed, the temperature or flow rate of the salt can be varied based on information from a temperature sensor, most likely a thermocouple on the pre-heating stream (S-512), to achieve the desired cold stream (S-600) outlet temperature.

The reactor outlet (S-601) must be cooled to an appropriate temperature to reenter the distillation columns. This control can be fairly loose, as the column design is robust enough to
handle a moderate range of entry conditions. However, if necessary the flow rate of cooling water (CW-600) through the final post-transalkylation heat exchanger (HW-601) can be varied to ensure an appropriate temperature based on information obtained from a temperature sensor, most likely a thermocouple on the post-heat-recovery transalkylation product stream (S-602).

Section 700: Furnace

In Section 700, the outlet temperatures and flow rates of the Dowtherm A (S-719), process steam (S-727), and molten salt (S-723) streams must be controlled such that they provide the necessary heat duties in other sections of the process. This will rely on data from a variety of temperature sensors, most likely thermocouples, placed on the cold stream feeds entering each heat exchanger that uses these heating streams. The system will also require thermocouples on each exiting stream (S-719, S-723, and S-727) in order to ensure proper exit temperatures. Alternatively and more likely, given the high temperatures these streams reach, the flow rates, rather than the temperatures, will be controlled in by valves in response to temperature data from the thermocouples.

In order to control the outlet temperatures, data from the thermocouples will also be sent to valves located in the combined waste stream (S-700). These valves will divert the flow of flammable waste in order to achieve the required heating duties. A holdup tank within the combined stream (S-700) will likely be necessary in order to enable the desired level of control over burn rates. In addition, this tank may need to have supplemental fuel feeds available to counter unexpected energy losses. Overall, this section represents the most complex system of interrelated controls and responses in the process; designers should build in as much flexibility as possible in order to enable successful operation of control systems implemented elsewhere in the process.

Safety Considerations
Many of the materials used in this process are highly flammable such as hydrocarbons and hydrogen. Extreme care must be exercised, despite the lack of oxygen in the feed streams, because of the possibility of an explosion caused by a leak. For this reason open flames and sparks should not be permitted anywhere near the hydrogenation, condensation, aqueous phase reforming, transalkylation and separation processes in particular. Emergency shut-off valves should be installed into the process to prevent large scale accidents. Nitrogen should be used to flush pipes of any combustible residue when performing catalyst recharge or cleaning.

In addition to the risks of explosions and fires due to the large amounts of hydrocarbons flowing through the system, hydrocarbon gases often present health risks via inhalation. For this reason, prolonged exposure to gases should be avoided at all costs. Additionally, risks of incomplete combustion within the furnaces could produce carbon monoxide. Carbon monoxide is very hazardous as it is both highly flammable and quite deadly if inhaled. Carbon dioxide also poses health risks if inhaled in large quantities. For these reasons, contact with the furnace should be avoided.

Many of the reactors are require high temperatures and pressures to react so reactors that can withstand intense conditions must be used. For this reason, contact with any of the reactors or heated streams should be avoided to prevent burns.

São Paulo, Brazil is known for its highly unreliable weather as it can vary drastically from day to day. It is also the location of tremendous amounts of rainfall. For this reason much of the pipes and equipment should be made of stainless steel to avoid corrosion and rusting particularly if it is to be kept outdoors.
Section VIII
Process Economics
VIII. PROCESS ECONOMICS

At a p-xylene price of $0.83/lb, a benzene price of $0.45/lb, and a sugar cane molasses price of $0.03/lb, this process is unprofitable, with an ROI of -2.90%. Profitability measures are summarized in Figure 16. The inputs leading up to these findings are described in the following sections: overview and materials, equipment cost estimates, utility requirements, cost summaries, and cash flows. This section concludes with a series of sensitivity analyses. Although profitability is feasible under certain conditions, the primary hurdle is that of overall conversion. Given the already optimistic assumptions throughout the process, making this investment is not recommended without technological advances. Namely, unless overall conversion can increase from 4.3% to 5.6%, the outlay is undesirable.

Figure 16

<table>
<thead>
<tr>
<th>Profitability Measures</th>
</tr>
</thead>
<tbody>
<tr>
<td>The Internal Rate of Return (IRR) for this project is</td>
</tr>
<tr>
<td>The Net Present Value (NPV) of this project in 2012 is</td>
</tr>
</tbody>
</table>

ROI Analysis (Third Production Year)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual Sales</td>
<td>297,083,393</td>
</tr>
<tr>
<td>Annual Costs</td>
<td>(287,852,062)</td>
</tr>
<tr>
<td>Depreciation</td>
<td>(23,039,899)</td>
</tr>
<tr>
<td>Income Tax</td>
<td>4,768,542</td>
</tr>
<tr>
<td>Net Earnings</td>
<td>(9,140,111)</td>
</tr>
<tr>
<td>Total Capital Investment</td>
<td>315,266,337</td>
</tr>
<tr>
<td>ROI</td>
<td>2.99%</td>
</tr>
</tbody>
</table>

Overview & Materials

Due to the choice of sugar cane molasses as a primary input, the process would be located in Brazil. A site factor of 0.85 is chosen as representative of the BRIC countries (Table 22.13, PPDP). Allowing for 35 days per year of down time, an operating factor of 0.9041 is selected. Therefore, 50,505 lb/h of p-xylene is required to achieve the requisite 400,000,000 lb/y. One year is permitted for design and for construction. Under the assumption that standard bulk contract pricing applies,
prices of $1,818/MT, $1,001/MT, and $60/MT are used for p-xylene, benzene (ICIS), and sugar cane molasses. These prices have a large impact on bottom-line profit and tend to fluctuate widely. Their impact is examined in the sensitivity analyses.
## General Information

Process Title: **P-Xylene from Sugar Cane Molasses**  
Product: **Para-Xylene**  
Plant Site Location: **Brazil**  
Site Factor: **0.85**  
Operating Hours per Year: **7920**  
Operating Days Per Year: **330**  
Operating Factor: **0.9041**

## Product Information

This Process will Yield  
- **50,505 lb** of Para-Xylene per hour  
- **1,212,121 lb** of Para-Xylene per day  
- **400,000,000 lb** of Para-Xylene per year  

Price  
- $0.83 /lb

## Chronology

<table>
<thead>
<tr>
<th>Year</th>
<th>Action</th>
<th>Distribution of Permanent Investment</th>
<th>Production Capacity</th>
<th>Depreciation 5 year MACRS</th>
<th>Product Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012</td>
<td>Design</td>
<td>0.0%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2013</td>
<td>Construction</td>
<td>100%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2014</td>
<td>Production</td>
<td>0%</td>
<td>45.0%</td>
<td>20.00%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2015</td>
<td>Production</td>
<td>0%</td>
<td>57.5%</td>
<td>32.00%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2016</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>19.20%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2017</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>11.52%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2018</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>11.52%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2019</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td>5.76%</td>
<td>$0.83</td>
</tr>
<tr>
<td>2020</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td></td>
<td>$0.83</td>
</tr>
<tr>
<td>2021</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td></td>
<td>$0.83</td>
</tr>
<tr>
<td>2022</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td></td>
<td>$0.83</td>
</tr>
<tr>
<td>2023</td>
<td>Production</td>
<td>0%</td>
<td>90.0%</td>
<td></td>
<td>$0.83</td>
</tr>
<tr>
<td>2043</td>
<td>Production</td>
<td>90.0%</td>
<td></td>
<td></td>
<td>$0.83</td>
</tr>
</tbody>
</table>
Equipment Cost Estimates

Equipment costs represent a large portion of the overall initial capital investment, totaling over $230 million. The largest expenditure categories are catalysts, heat exchange equipment, and storage vessels. Most equipment prices are reported according to ASPEN IPE estimates. Catalysts are discussed throughout the unit descriptions. Storage vessels, one heat exchanger, and furnaces are priced using the equations of Table 22.32 in PPDP – details are reported in the respective sections. Figure 17 summarizes equipment expenditure by type. Storage and catalyst are two significant costs that should be first priorities for cost reduction. Storage is especially significant because it also represents a large opportunity cost (two-thirds of storage vessels are unused for three-quarters of the year, for example – see Section 700.

Figure 17

![Equipment Costs by Type](image)

Note that “hand-priced” equipment was adjusted for the change in the Chemical Engineering Cost Index (data from Table 22.6, PPDP), extrapolation shown in Figure 18. Statistically speaking, predictive extrapolation is extremely dangerous; however, there was little other choice available. The period from 2002-2006 appears to be a “new normal,” and, if this assumption holds, the
extrapolation will not be far off the true value. That said, it is likely that the financial events since 2008 have had a negative impact on the CE growth. Fortunately, this affects a small number of units.

Figure 18
## Equipment Cost Summary

<table>
<thead>
<tr>
<th>Equipment Description</th>
<th>Bare Module Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure Changers</td>
<td>$16,259,900</td>
</tr>
<tr>
<td>Phase Changers</td>
<td>$2,586,900</td>
</tr>
<tr>
<td>Heat Exchangers</td>
<td>$33,421,700</td>
</tr>
<tr>
<td>Reactors</td>
<td>$5,923,400</td>
</tr>
<tr>
<td>Separations Equipment</td>
<td>$20,022,400</td>
</tr>
<tr>
<td>Storage Vessels</td>
<td>$31,887,500</td>
</tr>
<tr>
<td>Up-Front Utilities</td>
<td>$5,368,660</td>
</tr>
<tr>
<td>Catalyst</td>
<td>$117,586,508</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$233,068,868</strong></td>
</tr>
</tbody>
</table>
### Equipment Cost Details

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Purchase Cost</th>
<th>Bare Module Factor</th>
<th>Bare Module Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNF-300</td>
<td>Process Machinery</td>
<td>$10,132,800</td>
<td>1.1</td>
<td>$10,988,300</td>
</tr>
<tr>
<td>CNO-600</td>
<td>Fabricated Equipment</td>
<td>$33,600</td>
<td>3.4</td>
<td>$115,500</td>
</tr>
<tr>
<td>AD-500</td>
<td>Fabricated Equipment</td>
<td>$27,700</td>
<td>6.7</td>
<td>$155,500</td>
</tr>
<tr>
<td>RG-500</td>
<td>Fabricated Equipment</td>
<td>$361,200</td>
<td>1.5</td>
<td>$555,700</td>
</tr>
<tr>
<td>DP-800</td>
<td>Process Machinery</td>
<td>$9,900</td>
<td>5.8</td>
<td>$67,700</td>
</tr>
<tr>
<td>DC-500</td>
<td>Fabricated Equipment</td>
<td>$258,900</td>
<td>2.0</td>
<td>$1,050,200</td>
</tr>
<tr>
<td>CN-601</td>
<td>Fabricated Equipment</td>
<td>$31,600</td>
<td>3.7</td>
<td>$111,300</td>
</tr>
<tr>
<td>AD-501</td>
<td>Fabricated Equipment</td>
<td>$35,100</td>
<td>5.1</td>
<td>$180,000</td>
</tr>
<tr>
<td>RG-601</td>
<td>Fabricated Equipment</td>
<td>$238,100</td>
<td>1.6</td>
<td>$371,300</td>
</tr>
<tr>
<td>DP-801</td>
<td>Process Machinery</td>
<td>$13,600</td>
<td>4.9</td>
<td>$67,200</td>
</tr>
<tr>
<td>DC-501</td>
<td>Fabricated Equipment</td>
<td>$450,000</td>
<td>2.0</td>
<td>$900,000</td>
</tr>
<tr>
<td>CNC-602</td>
<td>Fabricated Equipment</td>
<td>$215,100</td>
<td>1.6</td>
<td>$340,300</td>
</tr>
<tr>
<td>AD-502</td>
<td>Fabricated Equipment</td>
<td>$51,600</td>
<td>3.9</td>
<td>$195,500</td>
</tr>
<tr>
<td>RS-602</td>
<td>Fabricated Equipment</td>
<td>$312,700</td>
<td>1.7</td>
<td>$522,000</td>
</tr>
<tr>
<td>DP-802</td>
<td>Process Machinery</td>
<td>$28,600</td>
<td>3.9</td>
<td>$104,200</td>
</tr>
<tr>
<td>DC-502</td>
<td>Fabricated Equipment</td>
<td>$580,000</td>
<td>2.2</td>
<td>$1,278,500</td>
</tr>
<tr>
<td>CN-603</td>
<td>Fabricated Equipment</td>
<td>$205,100</td>
<td>1.6</td>
<td>$421,200</td>
</tr>
<tr>
<td>AD-503</td>
<td>Fabricated Equipment</td>
<td>$18,700</td>
<td>6.7</td>
<td>$126,000</td>
</tr>
<tr>
<td>RS-503</td>
<td>Fabricated Equipment</td>
<td>$29,600</td>
<td>3.6</td>
<td>$113,500</td>
</tr>
<tr>
<td>DP-603</td>
<td>Process Machinery</td>
<td>$6,200</td>
<td>6.3</td>
<td>$39,000</td>
</tr>
<tr>
<td>DC-503</td>
<td>Fabricated Equipment</td>
<td>$117,600</td>
<td>2.6</td>
<td>$330,800</td>
</tr>
<tr>
<td>F-300</td>
<td>Fabricated Equipment</td>
<td>$35,100</td>
<td>4.1</td>
<td>$142,900</td>
</tr>
<tr>
<td>F-301</td>
<td>Fabricated Equipment</td>
<td>$24,600</td>
<td>4.5</td>
<td>$157,400</td>
</tr>
<tr>
<td>HX-100</td>
<td>Fabricated Equipment</td>
<td>$51,200</td>
<td>4.4</td>
<td>$225,000</td>
</tr>
<tr>
<td>HX-101</td>
<td>Fabricated Equipment</td>
<td>$51,200</td>
<td>4.4</td>
<td>$225,000</td>
</tr>
<tr>
<td>HX-102</td>
<td>Fabricated Equipment</td>
<td>$51,200</td>
<td>4.4</td>
<td>$225,000</td>
</tr>
<tr>
<td>HX-200</td>
<td>Fabricated Equipment</td>
<td>$206,600</td>
<td>1.7</td>
<td>$498,300</td>
</tr>
<tr>
<td>HX-300</td>
<td>Fabricated Equipment</td>
<td>$56,000</td>
<td>3.1</td>
<td>$174,400</td>
</tr>
<tr>
<td>HX-301</td>
<td>Fabricated Equipment</td>
<td>$174,200</td>
<td>1.9</td>
<td>$338,000</td>
</tr>
<tr>
<td>HX-302</td>
<td>Fabricated Equipment</td>
<td>$16,000</td>
<td>5.2</td>
<td>$83,100</td>
</tr>
<tr>
<td>HX-303</td>
<td>Fabricated Equipment</td>
<td>$195,100</td>
<td>1.5</td>
<td>$347,500</td>
</tr>
<tr>
<td>HX-400</td>
<td>Fabricated Equipment</td>
<td>$156,000</td>
<td>4.0</td>
<td>$716,100</td>
</tr>
<tr>
<td>HX-401</td>
<td>Fabricated Equipment</td>
<td>$334,400</td>
<td>1.6</td>
<td>$1,375,300</td>
</tr>
<tr>
<td>HX-402</td>
<td>Fabricated Equipment</td>
<td>$39,400</td>
<td>3.5</td>
<td>$130,400</td>
</tr>
<tr>
<td>HX-403</td>
<td>Fabricated Equipment</td>
<td>$383,200</td>
<td>2.0</td>
<td>$767,900</td>
</tr>
<tr>
<td>HX-404</td>
<td>Fabricated Equipment</td>
<td>$3,569,500</td>
<td>3.2</td>
<td>$11,384,800</td>
</tr>
<tr>
<td>HX-500</td>
<td>Fabricated Equipment</td>
<td>$54,200</td>
<td>2.6</td>
<td>$150,200</td>
</tr>
<tr>
<td>HX-601</td>
<td>Fabricated Equipment</td>
<td>$24,200</td>
<td>4.0</td>
<td>$96,000</td>
</tr>
<tr>
<td>HX-600</td>
<td>Fabricated Equipment</td>
<td>$66,700</td>
<td>5.6</td>
<td>$341,900</td>
</tr>
<tr>
<td>HX-601</td>
<td>Fabricated Equipment</td>
<td>$34,600</td>
<td>3.4</td>
<td>$115,400</td>
</tr>
<tr>
<td>HX-703</td>
<td>Fabricated Equipment</td>
<td>$22,700</td>
<td>4.8</td>
<td>$197,800</td>
</tr>
<tr>
<td>HX-704</td>
<td>Fabricated Equipment</td>
<td>$24,700</td>
<td>4.6</td>
<td>$197,600</td>
</tr>
<tr>
<td>P-300</td>
<td>Process Machinery</td>
<td>$11,400</td>
<td>7.4</td>
<td>$84,300</td>
</tr>
<tr>
<td>P-301</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-302</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-303</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-304</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-305</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-306</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-307</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>P-308</td>
<td>Process Machinery</td>
<td>$10,200</td>
<td>5.6</td>
<td>$57,600</td>
</tr>
<tr>
<td>Name (cont'd)</td>
<td>Type</td>
<td>Purchase Cost</td>
<td>Bare Module Factor</td>
<td>Bare Module Cost</td>
</tr>
<tr>
<td>--------------</td>
<td>-----------------------</td>
<td>---------------</td>
<td>--------------------</td>
<td>------------------</td>
</tr>
<tr>
<td>P-200</td>
<td>Process Machinery</td>
<td>$6,500</td>
<td>8.1</td>
<td>$52,800</td>
</tr>
<tr>
<td>P-210</td>
<td>Process Machinery</td>
<td>$6,500</td>
<td>8.1</td>
<td>$52,800</td>
</tr>
<tr>
<td>P-211</td>
<td>Process Machinery</td>
<td>$6,500</td>
<td>8.1</td>
<td>$52,800</td>
</tr>
<tr>
<td>P-300</td>
<td>Process Machinery</td>
<td>$6,500</td>
<td>6.8</td>
<td>$47,000</td>
</tr>
<tr>
<td>P-301</td>
<td>Process Machinery</td>
<td>$6,000</td>
<td>7.5</td>
<td>$45,000</td>
</tr>
<tr>
<td>P-302</td>
<td>Process Machinery</td>
<td>$6,400</td>
<td>6.9</td>
<td>$57,700</td>
</tr>
<tr>
<td>P-400</td>
<td>Process Machinery</td>
<td>$10,600</td>
<td>11.3</td>
<td>$118,300</td>
</tr>
<tr>
<td>P-401</td>
<td>Process Machinery</td>
<td>$13,400</td>
<td>20.3</td>
<td>$272,300</td>
</tr>
<tr>
<td>P-402</td>
<td>Process Machinery</td>
<td>$11,000</td>
<td>11.0</td>
<td>$121,400</td>
</tr>
<tr>
<td>P-500</td>
<td>Process Machinery</td>
<td>$6,000</td>
<td>6.5</td>
<td>$45,200</td>
</tr>
<tr>
<td>P-501</td>
<td>Process Machinery</td>
<td>$7,400</td>
<td>7.2</td>
<td>$53,600</td>
</tr>
<tr>
<td>P-502</td>
<td>Process Machinery</td>
<td>$7,200</td>
<td>7.4</td>
<td>$53,500</td>
</tr>
<tr>
<td>P-505</td>
<td>Process Machinery</td>
<td>$5,100</td>
<td>6.7</td>
<td>$54,000</td>
</tr>
<tr>
<td>P-506</td>
<td>Process Machinery</td>
<td>$7,900</td>
<td>6.5</td>
<td>$54,200</td>
</tr>
<tr>
<td>P-700</td>
<td>Process Machinery</td>
<td>$51,300</td>
<td>8.4</td>
<td>$421,700</td>
</tr>
<tr>
<td>P-701</td>
<td>Process Machinery</td>
<td>$51,300</td>
<td>9.4</td>
<td>$421,700</td>
</tr>
<tr>
<td>P-702</td>
<td>Process Machinery</td>
<td>$75,600</td>
<td>11.3</td>
<td>$854,100</td>
</tr>
<tr>
<td>P-703</td>
<td>Process Machinery</td>
<td>$27,100</td>
<td>4.2</td>
<td>$114,000</td>
</tr>
<tr>
<td>P-704</td>
<td>Process Machinery</td>
<td>$11,900</td>
<td>7.3</td>
<td>$84,100</td>
</tr>
<tr>
<td>P-705</td>
<td>Process Machinery</td>
<td>$4,500</td>
<td>7.9</td>
<td>$35,400</td>
</tr>
<tr>
<td>P-705/N</td>
<td>Process Machinery</td>
<td>$4,500</td>
<td>7.9</td>
<td>$35,400</td>
</tr>
<tr>
<td>P-705-Z</td>
<td>Process Machinery</td>
<td>$4,500</td>
<td>7.9</td>
<td>$35,400</td>
</tr>
<tr>
<td>P-705/N-Z</td>
<td>Process Machinery</td>
<td>$4,500</td>
<td>7.9</td>
<td>$35,400</td>
</tr>
<tr>
<td>P-706</td>
<td>Process Machinery</td>
<td>$5,200</td>
<td>7.8</td>
<td>$40,500</td>
</tr>
<tr>
<td>P-706/N</td>
<td>Process Machinery</td>
<td>$5,200</td>
<td>7.8</td>
<td>$40,500</td>
</tr>
<tr>
<td>P-707</td>
<td>Process Machinery</td>
<td>$4,700</td>
<td>7.8</td>
<td>$35,600</td>
</tr>
<tr>
<td>P-707/N</td>
<td>Process Machinery</td>
<td>$4,700</td>
<td>7.8</td>
<td>$35,600</td>
</tr>
<tr>
<td>P-708</td>
<td>Process Machinery</td>
<td>$6,300</td>
<td>7.0</td>
<td>$43,800</td>
</tr>
<tr>
<td>P-708/N</td>
<td>Process Machinery</td>
<td>$6,300</td>
<td>7.0</td>
<td>$43,800</td>
</tr>
<tr>
<td>P-709</td>
<td>Process Machinery</td>
<td>$6,300</td>
<td>7.0</td>
<td>$43,800</td>
</tr>
<tr>
<td>P-709/N</td>
<td>Process Machinery</td>
<td>$6,300</td>
<td>7.0</td>
<td>$43,800</td>
</tr>
<tr>
<td>R-100</td>
<td>Fabricated Equipment</td>
<td>$179,100</td>
<td>1.3</td>
<td>$338,800</td>
</tr>
<tr>
<td>R-101</td>
<td>Fabricated Equipment</td>
<td>$179,100</td>
<td>1.3</td>
<td>$338,800</td>
</tr>
<tr>
<td>R-102</td>
<td>Fabricated Equipment</td>
<td>$179,100</td>
<td>1.3</td>
<td>$338,800</td>
</tr>
<tr>
<td>R-200</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-201</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-202</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-203</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-204</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-205</td>
<td>Fabricated Equipment</td>
<td>$191,300</td>
<td>1.5</td>
<td>$348,800</td>
</tr>
<tr>
<td>R-300</td>
<td>Fabricated Equipment</td>
<td>$233,300</td>
<td>2.0</td>
<td>$460,500</td>
</tr>
<tr>
<td>R-400</td>
<td>Fabricated Equipment</td>
<td>$233,300</td>
<td>2.0</td>
<td>$460,500</td>
</tr>
<tr>
<td>R-401</td>
<td>Fabricated Equipment</td>
<td>$233,300</td>
<td>2.0</td>
<td>$460,500</td>
</tr>
<tr>
<td>R-402</td>
<td>Fabricated Equipment</td>
<td>$233,300</td>
<td>2.0</td>
<td>$460,500</td>
</tr>
<tr>
<td>R-403</td>
<td>Fabricated Equipment</td>
<td>$233,300</td>
<td>2.0</td>
<td>$460,500</td>
</tr>
<tr>
<td>R-500</td>
<td>Fabricated Equipment</td>
<td>$310,600</td>
<td>1.3</td>
<td>$467,800</td>
</tr>
</tbody>
</table>
### Section VIII: Process Economics

<table>
<thead>
<tr>
<th>Name (cont’d)</th>
<th>Type</th>
<th>Purchase Cost</th>
<th>Bare Module Factor</th>
<th>Bare Module Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>FRN-700</td>
<td>Fabricated Equipment</td>
<td>$1,626,600</td>
<td>2.0</td>
<td>$3,253,200</td>
</tr>
<tr>
<td>FRN-701</td>
<td>Fabricated Equipment</td>
<td>$5,186,600</td>
<td>1.0</td>
<td>$5,186,600</td>
</tr>
<tr>
<td>FRN-702</td>
<td>Fabricated Equipment</td>
<td>$5,186,600</td>
<td>1.0</td>
<td>$5,186,600</td>
</tr>
<tr>
<td>FRN-703</td>
<td>Fabricated Equipment</td>
<td>$1,495,600</td>
<td>1.0</td>
<td>$1,495,600</td>
</tr>
<tr>
<td>CRY-500</td>
<td>Fabricated Equipment</td>
<td>$15,000,000</td>
<td>1.0</td>
<td>$15,000,000</td>
</tr>
<tr>
<td>WC-500</td>
<td>Fabricated Equipment</td>
<td>-</td>
<td>-</td>
<td>**</td>
</tr>
<tr>
<td>SEP-300</td>
<td>Fabricated Equipment</td>
<td>$52,000</td>
<td>3.9</td>
<td>$202,700</td>
</tr>
<tr>
<td>SEP-300</td>
<td>Fabricated Equipment</td>
<td>$30,100</td>
<td>5.8</td>
<td>$173,300</td>
</tr>
<tr>
<td>SEP-501</td>
<td>Fabricated Equipment</td>
<td>$21,900</td>
<td>6.5</td>
<td>$142,100</td>
</tr>
<tr>
<td>ST-000</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-001</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-002</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-003</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-004</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-005</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-006</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-007</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-008</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-009</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-010</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-011</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-012</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-013</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-014</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-015</td>
<td>Storage</td>
<td>-</td>
<td>-</td>
<td>$1,906,800</td>
</tr>
<tr>
<td>ST-700</td>
<td>Storage</td>
<td>$599,300</td>
<td>1.2</td>
<td>$719,900</td>
</tr>
<tr>
<td>ST-701</td>
<td>Storage</td>
<td>$329,400</td>
<td>2.0</td>
<td>$658,800</td>
</tr>
<tr>
<td>CAT-100</td>
<td>Catalysts</td>
<td>-</td>
<td>-</td>
<td>**</td>
</tr>
<tr>
<td>CAT-200</td>
<td>Catalysts</td>
<td>-</td>
<td>-</td>
<td>$15,391,073</td>
</tr>
<tr>
<td>CAT-300</td>
<td>Catalysts</td>
<td>-</td>
<td>-</td>
<td>$17,995,528</td>
</tr>
<tr>
<td>CAT-400</td>
<td>Catalysts</td>
<td>-</td>
<td>-</td>
<td>$11,744,983</td>
</tr>
<tr>
<td>CAT-500</td>
<td>Catalysts</td>
<td>-</td>
<td>-</td>
<td>$6,065,743</td>
</tr>
<tr>
<td>S-720*</td>
<td>Other Equipment</td>
<td>-</td>
<td>-</td>
<td>$3,793,160</td>
</tr>
<tr>
<td>S-721*</td>
<td>Other Equipment</td>
<td>-</td>
<td>-</td>
<td>$1,575,500</td>
</tr>
</tbody>
</table>

*One-time heating fluid purchases **The washing column is included in the cryogenic freezer's purchase price.
Utility Requirements

The utility cost for the plant is calculated using prices from Table 23.1 of PPDP, and the utility requirements as derived from ASPEN or as calculated according to various heating requirements. More information on utilities can be found in Section IV: Energy Balance.
### Section VIII: Process Economics

#### Utility Costs

<table>
<thead>
<tr>
<th>Utility</th>
<th>Name</th>
<th>Energy Requirement (kW)</th>
<th>Rate</th>
<th>Cost (Annual)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Price: $0.060/kWh</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CMP-300</td>
<td>16659.17</td>
<td>-</td>
<td></td>
<td>$7,916,437.58</td>
</tr>
<tr>
<td>DP-500</td>
<td>149.14</td>
<td>-</td>
<td></td>
<td>$70,871.33</td>
</tr>
<tr>
<td>DP-501</td>
<td>111.85</td>
<td>-</td>
<td></td>
<td>$53,151.12</td>
</tr>
<tr>
<td>DP-502</td>
<td>186.42</td>
<td>-</td>
<td></td>
<td>$88,586.78</td>
</tr>
<tr>
<td>DP-503</td>
<td>55.93</td>
<td>-</td>
<td></td>
<td>$26,577.94</td>
</tr>
<tr>
<td>P-000</td>
<td>2.23</td>
<td>-</td>
<td></td>
<td>$1,058.97</td>
</tr>
<tr>
<td>P-100</td>
<td>10.54</td>
<td>-</td>
<td></td>
<td>$5,008.57</td>
</tr>
<tr>
<td>P-101</td>
<td>10.84</td>
<td>-</td>
<td></td>
<td>$5,151.67</td>
</tr>
<tr>
<td>P-102</td>
<td>10.84</td>
<td>-</td>
<td></td>
<td>$5,151.67</td>
</tr>
<tr>
<td>P-103</td>
<td>491.50</td>
<td>-</td>
<td></td>
<td>$233,559.91</td>
</tr>
<tr>
<td>P-104</td>
<td>491.50</td>
<td>-</td>
<td></td>
<td>$233,559.91</td>
</tr>
<tr>
<td>P-105</td>
<td>491.50</td>
<td>-</td>
<td></td>
<td>$233,559.91</td>
</tr>
<tr>
<td>P-200</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-201</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-202</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-203</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-204</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-205</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-206</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-207</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-208</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-209</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-210</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-211</td>
<td>0.45</td>
<td>-</td>
<td></td>
<td>$213.84</td>
</tr>
<tr>
<td>P-300</td>
<td>2.53</td>
<td>-</td>
<td></td>
<td>$1,200.39</td>
</tr>
<tr>
<td>P-301</td>
<td>0.25</td>
<td>-</td>
<td></td>
<td>$118.80</td>
</tr>
<tr>
<td>P-302</td>
<td>1.78</td>
<td>-</td>
<td></td>
<td>$845.81</td>
</tr>
<tr>
<td>P-400</td>
<td>1.86</td>
<td>-</td>
<td></td>
<td>$884.06</td>
</tr>
<tr>
<td>P-401</td>
<td>2.94</td>
<td>-</td>
<td></td>
<td>$1,397.42</td>
</tr>
<tr>
<td>P-402</td>
<td>1.96</td>
<td>-</td>
<td></td>
<td>$936.63</td>
</tr>
<tr>
<td>P-500</td>
<td>1.95</td>
<td>-</td>
<td></td>
<td>$926.64</td>
</tr>
<tr>
<td>P-501</td>
<td>0.47</td>
<td>-</td>
<td></td>
<td>$229.53</td>
</tr>
<tr>
<td>P-502</td>
<td>0.55</td>
<td>-</td>
<td></td>
<td>$261.55</td>
</tr>
<tr>
<td>P-503</td>
<td>0.23</td>
<td>-</td>
<td></td>
<td>$111.19</td>
</tr>
<tr>
<td>P-601</td>
<td>0.67</td>
<td>-</td>
<td></td>
<td>$316.26</td>
</tr>
<tr>
<td>P-700</td>
<td>92.10</td>
<td>-</td>
<td></td>
<td>$43,765.92</td>
</tr>
<tr>
<td>P-701</td>
<td>92.10</td>
<td>-</td>
<td></td>
<td>$43,765.92</td>
</tr>
<tr>
<td>P-702</td>
<td>29.65</td>
<td>-</td>
<td></td>
<td>$14,089.68</td>
</tr>
<tr>
<td>P-703</td>
<td>87.74</td>
<td>-</td>
<td></td>
<td>$41,694.05</td>
</tr>
</tbody>
</table>
# Utility Costs (2/2)

<table>
<thead>
<tr>
<th></th>
<th>(Unit)</th>
<th>(MBtu/h)</th>
<th>(gal/min)</th>
<th>(Annual)</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-704</td>
<td>2.49</td>
<td>-</td>
<td>$1,183.25</td>
<td></td>
</tr>
<tr>
<td>P-705</td>
<td>0.14</td>
<td>-</td>
<td>$65.45</td>
<td></td>
</tr>
<tr>
<td>P-705IN</td>
<td>0.21</td>
<td>-</td>
<td>$98.18</td>
<td></td>
</tr>
<tr>
<td>P-706</td>
<td>0.25</td>
<td>-</td>
<td>$119.38</td>
<td></td>
</tr>
<tr>
<td>P-706IN</td>
<td>0.38</td>
<td>-</td>
<td>$179.07</td>
<td></td>
</tr>
<tr>
<td>P-707</td>
<td>0.17</td>
<td>-</td>
<td>$81.53</td>
<td></td>
</tr>
<tr>
<td>P-707IN</td>
<td>0.26</td>
<td>-</td>
<td>$122.30</td>
<td></td>
</tr>
<tr>
<td>P-708</td>
<td>0.47</td>
<td>-</td>
<td>$224.19</td>
<td></td>
</tr>
<tr>
<td>P-708IN</td>
<td>0.63</td>
<td>-</td>
<td>$297.80</td>
<td></td>
</tr>
<tr>
<td>P-709</td>
<td>0.08</td>
<td>-</td>
<td>$37.28</td>
<td></td>
</tr>
<tr>
<td>P-709IN</td>
<td>0.12</td>
<td>-</td>
<td>$55.92</td>
<td></td>
</tr>
<tr>
<td>WC-500</td>
<td>1118.18</td>
<td>-</td>
<td>$531,359.14</td>
<td></td>
</tr>
</tbody>
</table>

**Total Electricity:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooling Water</td>
<td>(Unit)</td>
<td>(MBtu/h)</td>
<td>(gal/min)</td>
<td>(Annual)</td>
</tr>
<tr>
<td>Price: $0.075/kgal</td>
<td>HX-200</td>
<td>40.70</td>
<td>2,575.00</td>
<td>$91,773.00</td>
</tr>
<tr>
<td></td>
<td>HX-302</td>
<td>2.03</td>
<td>125.00</td>
<td>$4,455.00</td>
</tr>
<tr>
<td></td>
<td>HX-303</td>
<td>122.31</td>
<td>2,775.00</td>
<td>$98,901.00</td>
</tr>
<tr>
<td></td>
<td>HX-401</td>
<td>978.49</td>
<td>60,000.00</td>
<td>$2,138,400.00</td>
</tr>
<tr>
<td></td>
<td>CND-500</td>
<td>30.64</td>
<td>2,058.36</td>
<td>$73,360.12</td>
</tr>
<tr>
<td></td>
<td>CND-501</td>
<td>44.01</td>
<td>2,956.55</td>
<td>$105,371.38</td>
</tr>
<tr>
<td></td>
<td>CND-502</td>
<td>133.43</td>
<td>8,963.70</td>
<td>$319,466.10</td>
</tr>
<tr>
<td></td>
<td>CND-503</td>
<td>11.09</td>
<td>745.02</td>
<td>$26,552.34</td>
</tr>
<tr>
<td></td>
<td>CMP-300</td>
<td>30.56</td>
<td>2,052.99</td>
<td>$73,168.58</td>
</tr>
</tbody>
</table>

**Total Cooling Water:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Chilled Water</td>
<td>(Unit)</td>
<td>(ton-day)</td>
<td>(gal/min)</td>
<td>(Annual)</td>
</tr>
<tr>
<td>Price: $1.20/ton-day</td>
<td>HX-500</td>
<td>1011.25</td>
<td>1650.00</td>
<td>$600,682.50</td>
</tr>
<tr>
<td></td>
<td>HX-501</td>
<td>435.11</td>
<td>1000.00</td>
<td>$258,456.83</td>
</tr>
</tbody>
</table>

**Total Chilled Water:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Refrigeration</td>
<td>(Unit)</td>
<td>(ton-day)</td>
<td>(N/A)</td>
<td>(Annual)</td>
</tr>
<tr>
<td>Price: $3.10/ton-day</td>
<td>CRY-500</td>
<td>491.22</td>
<td>-</td>
<td>$502,518.24</td>
</tr>
</tbody>
</table>

**Total Refrigeration:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dowtherm A</td>
<td>(Stream)</td>
<td>(MBtu/h)</td>
<td>(lb)</td>
<td>(One-time)</td>
</tr>
<tr>
<td>Price: $7.13/lb</td>
<td>S-720</td>
<td>530.39</td>
<td>532,000.00</td>
<td>$3,793,160.00</td>
</tr>
</tbody>
</table>

**Total Dowtherm A:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Molten Salt</td>
<td>(Unit)</td>
<td>(MBtu/h)</td>
<td>(lb)</td>
<td>(One-time)</td>
</tr>
<tr>
<td>Price: $0.22/lb</td>
<td>HX-600</td>
<td>62.00</td>
<td>7,089,751.24</td>
<td>$1,575,500.28</td>
</tr>
</tbody>
</table>

**Total Molten Salt:**

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Utilities (Year 0):</td>
<td></td>
<td></td>
<td>$19,807,000.00</td>
<td></td>
</tr>
<tr>
<td>Total Recurring Utilities:</td>
<td></td>
<td></td>
<td>$14,438,000.00</td>
<td></td>
</tr>
</tbody>
</table>
Cost Summaries

Variable costs, working capital, fixed costs, and investment requirements are taken according to specifications in PPDP Table 23.1.

Working capital is taken to include four days of p-xylene inventory and 24 days of raw materials (four tanks of residence time six days not in use at any given time during peak production season).

Direct operating expenses total just over $7,000,000 per year, over 83% of which stems from wages and benefits. These wages and benefits are based on the operator wage of $35/h, which was fair in the United States in 2006, and still applies today in Brazil. The number of operators is determined from recommendations in Table 23.3 PPDP. The process has seven main sections, six of which are continuous fluids and one of which involves some solids handling. Therefore, at a scale of 610 tons per operating day, the recommended number of operators on-hand is 16: two for each fluids portion and four for the separations section that involves solids. This amounts to $6.7M per annum in wages, salary, and benefits.
**Variable Cost Summary**

**Variable Costs at 100% Capacity:**

**General Expenses**

- Selling / Transfer Expenses: $9,902,777
- Direct Research: $15,844,443
- Allocated Research: $1,650,463
- Administrative Expense: $6,801,351
- Management Incentive Compensation: $4,120,157

**Total General Expenses** $38,125,691

- **Raw Materials** $0.701410 per lb of Para-Xylene $280,564,139
- **Byproducts** $0.169315 per lb of Para-Xylene $(67,725,176)
- **Utilities** $0.033915 per lb of Para-Xylene $13,565,325

**Total Variable Costs** $264,529,970

**Working Capital**

<table>
<thead>
<tr>
<th></th>
<th>2013</th>
<th>2014</th>
<th>2015</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accounts Receivable</td>
<td>$12,206,863</td>
<td>$6,104,461</td>
<td>$6,104,461</td>
</tr>
<tr>
<td>Cash Reserves</td>
<td>$2,344,244</td>
<td>$1,172,122</td>
<td>$1,172,122</td>
</tr>
<tr>
<td>Accounts Payable</td>
<td>$(10,876,798)</td>
<td>$(5,439,309)</td>
<td>$(6,439,309)</td>
</tr>
<tr>
<td>Para-Xylene Inventory</td>
<td>$1,027,854</td>
<td>$813,927</td>
<td>$813,927</td>
</tr>
<tr>
<td>Raw Materials</td>
<td>$9,301,824</td>
<td>$4,150,912</td>
<td>$4,760,812</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$13,903,826</strong></td>
<td><strong>$8,031,913</strong></td>
<td><strong>$8,881,913</strong></td>
</tr>
</tbody>
</table>

**Present Value at 15%**

<table>
<thead>
<tr>
<th></th>
<th>2013</th>
<th>2014</th>
<th>2015</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>$11,029,414</td>
<td>$5,143,224</td>
<td>$4,472,305</td>
</tr>
</tbody>
</table>

**Total Capital Investment** $309,443,660
## Fixed Cost Summary

### Operations
- **Direct Wages and Benefits**: $5,824,000
- **Direct Salaries and Benefits**: $873,600
- **Operating Supplies and Services**: $349,440
- **Technical Assistance to Manufacturing**: $-
- **Control Laboratory**: $-

**Total Operations**: $7,047,040

### Maintenance
- **Wages and Benefits**: $13,613,383
- **Salaries and Benefits**: $3,403,346
- **Materials and Services**: $13,613,383
- **Maintenance Overhead**: $680,899

**Total Maintenance**: $31,310,781

### Operating Overhead
- **General Plant Overhead**: $1,663,717
- **Mechanical Department Services**: $569,144
- **Employee Relations Department**: $1,399,145
- **Business Services**: $1,754,860

**Total Operating Overhead**: $5,406,687

### Property Taxes and Insurance
- **Property Taxes and Insurance**: $6,050,393

### Other Annual Expenses
- **Rental Fees (Office and Laboratory Space)**: $-
- **Licensing Fees**: $-
- **Miscellaneous**: $-

**Total Other Annual Expenses**: $-

### Total Fixed Costs
- **Total Fixed Costs**: $49,815,081
## Investment Summary

### Bare Module Costs

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fabricated Equipment</td>
<td>$61,964,400</td>
</tr>
<tr>
<td>Process Machinery</td>
<td>$16,260,900</td>
</tr>
<tr>
<td>Spares</td>
<td>$-</td>
</tr>
<tr>
<td>Storage</td>
<td>$31,887,500</td>
</tr>
<tr>
<td>Other Equipment</td>
<td>$5,368,660</td>
</tr>
<tr>
<td>Catalysts</td>
<td>$117,585,508</td>
</tr>
<tr>
<td>Computers, Software, Etc.</td>
<td>$-</td>
</tr>
</tbody>
</table>

**Total Bare Module Costs:** $233,065,968

### Direct Permanent Investment

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Site Preparations</td>
<td>$11,653,298</td>
</tr>
<tr>
<td>Cost of Service Facilities</td>
<td>$11,653,298</td>
</tr>
<tr>
<td>Allocated Costs for utility plants and related facilities</td>
<td>$-</td>
</tr>
</tbody>
</table>

**Direct Permanent Investment:** $256,372,565

### Total Depreciable Capital

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Contingencies &amp; Contractor Fees</td>
<td>$46,147,062</td>
</tr>
</tbody>
</table>

**Total Depreciable Capital:** $302,519,626

### Total Permanent Investment

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Land</td>
<td>$6,050,383</td>
</tr>
<tr>
<td>Cost of Royalties</td>
<td>$-</td>
</tr>
<tr>
<td>Cost of Plant Start-Up</td>
<td>$30,251,963</td>
</tr>
</tbody>
</table>

**Total Permanent Investment - Unadjusted:** $338,821,982

**Site Factor:** 0.85

**Total Permanent Investment:** $287,998,864
Cash Flows

The most important features of the cash flow summary in this instance are the initial capital costs, the year of positive cash flow, and the ultimate NPV. The summary shows that, although the process becomes profitable in year seven of operation, the small cash flows (~$6M) never fully compensate for the large initial capital outlay, $288M. Ultimately, at a discount rate of 15%, which is conservative, the net present value of the process is $(196,282,500). This investment is not recommended under the given assumptions.
<table>
<thead>
<tr>
<th>Year</th>
<th>Percentage of Design Capacity</th>
<th>Product Unit Price</th>
<th>Sales</th>
<th>Capital Costs</th>
<th>Working Capital</th>
<th>Var Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012</td>
<td>0%</td>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2013</td>
<td>6%</td>
<td></td>
<td>-</td>
<td>(267,996,700)</td>
<td>(13,603,600)</td>
<td>-</td>
</tr>
<tr>
<td>2014</td>
<td>45%</td>
<td>$0.83</td>
<td>148,541,700</td>
<td>-</td>
<td>(6,801,900)</td>
<td>(119,038,500)</td>
</tr>
<tr>
<td>2015</td>
<td>69%</td>
<td>$0.83</td>
<td>222,612,500</td>
<td>-</td>
<td>(6,801,500)</td>
<td>(173,557,700)</td>
</tr>
<tr>
<td>2016</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2017</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2018</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2019</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2020</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2021</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2022</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2023</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2024</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2025</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2026</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2027</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2028</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2029</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2030</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2031</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2032</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2033</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2034</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2035</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2036</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2037</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2038</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2039</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2040</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2041</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2042</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>-</td>
<td>(238,077,000)</td>
</tr>
<tr>
<td>2043</td>
<td>90%</td>
<td>$0.83</td>
<td>297,083,300</td>
<td>-</td>
<td>27,207,700</td>
<td>(238,077,000)</td>
</tr>
</tbody>
</table>
### Cash Flow Summary [2/2]

<table>
<thead>
<tr>
<th></th>
<th>Fixed Costs</th>
<th>Depreciation</th>
<th>Taxable Income</th>
<th>Taxes</th>
<th>Net Earnings</th>
<th>Cash Flow</th>
<th>Cumulative Net Present Value at 15%</th>
</tr>
</thead>
<tbody>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(301,602,511)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td>(60,503,900)</td>
<td>(80,815,800)</td>
<td>27,477,400</td>
<td></td>
<td>(53,338,500)</td>
<td>363,554</td>
<td>(291,888,200)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(247,231,500)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(232,472,300)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(223,565,200)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(216,619,900)</td>
</tr>
<tr>
<td>(45,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(211,312,100)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(207,004,700)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(206,105,200)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(204,901,200)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(203,067,500)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(202,581,600)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(201,424,200)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(201,078,700)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(200,436,500)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(199,666,800)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(199,376,600)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(198,650,300)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(198,579,700)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(198,257,400)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,977,100)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,733,400)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,521,500)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,337,200)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,177,000)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(197,037,600)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(196,616,500)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(196,911,100)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(196,719,500)</td>
</tr>
<tr>
<td>(49,815,100)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(196,282,500)</td>
</tr>
</tbody>
</table>
Sensitivity Analyses

The most significant and the most variable cost and revenue drivers should always be examined for bottom-line impact, in order to be prepared for different operating scenarios. Key cost drivers of this process include the cost of sugar cane molasses, the price of electricity, the price of catalyst, and the overall conversion rate of molasses to p-xylene. Key revenue drivers include the price of p-xylene and the price of benzene.

IRR sensitivity tables are shown for product price against variable costs (Figure 19), fixed costs (Figure 20), and total permanent investment (Figure 21). These are rather generic measures intended to demonstrate the robustness of the assumptions detailed heretofore. Price fluctuations are taken at ±10%, which is reasonable given para-xylene’s recent performance and which is well within the norm of commodities markets.

More incisive sensitivity analyses are summarized in a Strauss plot, Figure 22 (Fig. 9-14, Perry’s).

Figure 19

<table>
<thead>
<tr>
<th>Product Price</th>
<th>Variable Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$230,075,981</td>
</tr>
<tr>
<td></td>
<td>$243,657,860</td>
</tr>
<tr>
<td></td>
<td>$248,855,180</td>
</tr>
<tr>
<td></td>
<td>$253,440,770</td>
</tr>
<tr>
<td></td>
<td>$258,239,379</td>
</tr>
<tr>
<td>$0.74</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.75</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.76</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.77</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.78</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.79</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.8</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.81</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.82</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.83</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.84</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.85</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.86</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.87</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.88</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.89</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.9</td>
<td>Negative IRR</td>
</tr>
<tr>
<td>$0.91</td>
<td>Negative IRR</td>
</tr>
</tbody>
</table>

This figure demonstrates relationship between product price (±10%) and variable cost (±10%). If product price were to increase any amount while variable cost either decreased or stayed constant, positive IRR would be achievable.
Section VIII: Process Economics

Figure 20

![Table](image)

This figure demonstrates relationship between product price (±10%) and fixed cost (±25%). If product price were to increase any amount while fixed cost either decreased or stayed constant, positive IRR would be achievable.

Figure 21

![Table](image)

This figure demonstrates relationship between product price (±10%) and total permanent investment (±50%). If product price were to increase any amount while TPI either decreased or stayed constant, positive IRR would be achievable.
This Strauss plot shows what percent change of which inputs would result in positive NPV. Notice, for example, that the effect of catalyst price is shown to be minimal at small price changes; however, if it increases to its full potential (see Catalyst), a 300% change, the effect could be devastating on profitability. It is clear that focus areas for improvement – those where positive NPV seems even feasible – should be the price of sugar cane molasses, the price of para-xylene, and the overall process conversion. Since the former two cannot be controlled, the best one can do is hedge against price fluctuations with futures contracts. Since the later is directly related to technological improvements, it makes sense to invest heavily in improving the overall process conversion. A 23%
increase in conversion – from the current 4.28% to a hopeful 5.55% - would achieve breakeven.

Incremental improvements above 5.55% overall conversion result in strongly positive NPV. This conversion is a clear and attainable goal, which would serve as a “green light” for the investment, if demonstrable.
Section IX
Conclusion & Recommendations
IX. CONCLUSION & RECOMMENDATIONS

Conclusion

At a para-xylene price of $0.83 per pound, a benzene price of $0.45 per pound, and a price for sugar cane molasses of $0.03 per pound, the renewable production of para-xylene is unprofitable, and earns a negative 2.90% return on investment (ROI). Furthermore, the net present value (NPV) of this project at a discount rate of 15% is a negative $196 million. This results from two facts. First, the process requires an initial investment of $309 million; this is difficult to recover given the time value of money. Second, while the process ultimately becomes cash flow positive, this only occurs after six years of operation, and expected yearly profits are only $6 million. These conclusions were reached using conservative assumptions; as such, construction of the process should not proceed.

However, the three key factors merit further research. The market for para-xylene still represents a great opportunity due to steadily growing demand, both renewable and in general (see Market Analysis). New findings in any of the three areas below would mitigate the low annual profits and possibly the high initial investment. The project could then proceed to a more rigorous design.

Recommendations

Recommendation 1: Reactor Yields

Overall, 23.38 pounds or molasses are consumed for every pound of para-xylene produced. This is a direct consequence of yields in the Aqueous Phase Reforming (APR) and Condensation sections (300 and 400, respectively) of the process. Even after recycling unconverted sorbitol, only 1.25% of sorbitol mass consumed by the APR is produced as hydrogen; the remainder consists of light hydrocarbons, which can be burned, and a major fraction of carbon-dioxide, which must simply be vented. In addition, only 8.27% of sorbitol consumed by the condensation reactions is produced as
para-xylene. Even increasing this yield by 27% via transalkylation results in only a 10.5% overall yield through the condensation and transalkylation combined.

However, these figures were conservatively restricted to specific examples found in patents and other relevant literature. Conditions in the aqueous phase reforming can likely be tailored to ensure full conversion of the leftover hydrocarbons to carbon dioxide and hydrogen; this would decrease the amount of additional feed required to supply hydrogen to the process. It is even more likely that the condensation reaction can be modified to generate a higher yield of para-xylene (currently only obtained in 46% of its theoretical yield). If both sections were to produce 100% of their theoretical hydrogen and para-xylene yields, the process would require 59.5% less molasses and save $167 million in raw materials costs every year. Decreasing the molasses costs by 23.2% of this 59.5%, which corresponds to increasing yields by 30% out of a potential 247%, causes the process to break even; any further advancement and the process returns a positive ROI and NPV.

**Recommendation 2: Catalysts**

The hydrolysis, hydrogenation, aqueous phase reforming, condensation, and transalkylation each require a substantial amount of zeolite catalyst. For most of these sections, no suitable catalysts were available for purchase. Instead, the process accounts for raw materials and manufacturing costs to provide the necessary catalysts. Following the advice of Professor Fabiano, we evaluated the process for three scenarios: raw material prices are not substantially lower in bulk than small quantities; raw material prices drop by 50% when purchased in bulk, and raw material prices drop by 25% when purchased in bulk. Due to the high cost of the raw materials, the process was modeled using the 25% price. Even so, the purchase and maintenance of the necessary amount of catalyst in perpetuity has a negative NPV of $117.6 million.

Further market and laboratory research is required to validate these pricing assumptions. It is possible that in large quantities the raw materials cost less than assumed, but the catalyst could also
cost significantly more. In the event that reactor yields can be improved, the catalyst costs must be
accurately estimated in order to ensure economic viability of the project.

If catalyst costs prove to be the deciding prohibitive factor, research into alternative catalyst
systems based on cheaper raw materials may be merited. Such research, if fruitful, would be
beneficial regardless of whether the renewable production of para-xylene was ultimately deemed
economically viable. If the process is to be constructed, the cheaper catalyst system would provide a
source of sustained competitive advantage. If not, the catalyst technology could be licensed to
incumbent producers of para-xylene, who no doubt also suffer from the high cost of their catalysts.

**Recommendation 3: Plant Acquisition and Reconstruction**

Even at low yields and high catalyst costs, the process ultimately generates $6 million in
profit per annum. However, this still represents a negative ROI and NPV due to the high amount of
initial investment necessary for this process. However, offsetting this cost would make the process
profitable as modeled in this report. One way to offset this cost would be the purchase and
repurposing of a similar plant. Condensation and transalkylation are fairly common practices in the
field, and it may be possible to acquire a facility with these capabilities already constructed.
Alternatively, the manufacture of sugar alcohols from biofuel materials as well as the production of
hydrogen via aqueous phase reforming are also reasonably common practices, either in separate or
combined plants. If available at a low price, purchasing an unwanted plant with one of these subset
of capabilities, then constructing the remaining sections of the plant necessary, could represent a
cheaper initial investment than construction from scratch.
Section X
Acknowledgments
X. ACKNOWLEDGMENTS

We would like to thank Professor Fabiano for organizing, overseeing, and providing guidance throughout the entire senior design process. We would also like to thank Dr. Wattenbarger, who advised us personally and provided a welcome source of support during the more strenuous periods of the project. We thank Mr. Stephen Tieri of DuPont, who wrote the initial problem statement, provided welcome guidance, and asked key questions at every turn. His constant availability was greatly appreciated. We are also indebted to every other consultant who sacrificed their time, effort, and energy on our behalf on a weekly basis; without these guiding hands, we would not have been able to handle the sheer magnitude of the problem we faced. All of these people share some stake of the credit for this report.

Thank you to our professors, Dr. Sean Holleran, Dr. Wen Shieh, Dr. Daeyeon Lee, Dr. John Vohs, Dr. Matthew Lazzara, Dr. Talid Sinno, Dr. John Crocker, and Dr. Warren Seider, for the time and effort put into our education over the last four years. Dr. Holleran, in particular, has served as a constant and welcome source of knowledge and advice throughout our Penn careers.

We also owe a very special thanks to Mrs. Meghan Godfrey, our friend in the CBE office, whose assistance made navigating the policies and procedures of the department, school, and university infinitely more bearable. She went above and beyond the call of duty at every turn, and we wish her and her newest family member the best. The CBE department is lucky to have Meghan on its team.
Section XI
Bibliography
XI. BIBLIOGRAPHY


SI Chemical Data Book (4th ed.), Gordon Aylward and Tristan Findlay, Jacaranda Wiley

Van Gorb, K., E. Boerman, C. V. Cavenaghi, and P. H. Berben. "Catalytic Hydrogenation of Fine

Section XII
Appendices
XII. APPENDICES

Appendix A: Problem Statement

Renewable Para-Xylene

The international demand for xylene isomers continues to increase steadily, with p-xylene in high demand as a key raw material in the bottling, packaging, materials, and fiber industries. Climate change, dwindling petroleum resources, a desire for energy independence, and consumer behavior are driving significant research and investment into the development of technologies that reduce energy consumption, improve efficiency, and produce chemicals and fuels from renewable resources. The disposition of agricultural resources and production to support both this transition from fossil to renewable fuels, while providing food to meet the demands of the increasing global population, is a source of controversy and significant discussion. Additionally, several beverage makers are actively seeking a plant-based route to plastics for their product packaging, to actively demonstrate their commitment to sustainability and the global environment.

Through its research efforts, your company has developed new and innovative technology to convert biomass-derived material into para-xylene, as an alternative to traditional production routes. Because the material from this innovative catalytic technology has the same composition as traditional petroleum-based para-xylene, it can be used directly in current manufacturing processes, or blended with conventional petroleum-based material, and distributed through existing supply chains without equipment modifications or separate shipping containers. In its current state, this technology is flexible to be optimized and modified to convert multiple renewable feedstocks to para-xylene, using a patented catalytic process to convert the plant-based sugars into monomer. In laboratory and pilot-scale testing, the technology has proven to be equally flexible with respect to potential raw materials, and able to accommodate a varying range of feed materials from glucose and sucrose (derived from sugar crops), starches, glycerol, polymers of glucose contained in cellulose (plant-cell walls), and longer chain C₅ and C₆ sugars (such as those contained in hemi-cellulose). Your company’s product trials show that the p-xylene produced using this technology is suitable for conversion into the polyethylene terephthalate (PET) raw material, purified terephthalic acid.

Your team has been assembled to design the first commercial facility, and to identify the optimal raw material to demonstrate the commercial viability of this new technology, using assumptions identified by your research and business directors. Your directors agree that the biomass options for this first facility should be limited to woody biomass, sugar cane, and corn grain. It's expected that woody biomass can be converted to sugars using standard enzymatic technology developed for the corn and cellulosic ethanol industry and available from industrial enzyme suppliers. However, they have concerns that the additional investment necessary for pre-treatment and enzymatic conversion of the biomass to sugars may restrict the economic viability of the innovation.

Your company recently acquired both corn dry-grind and sugar-cane ethanol facilities, in an effort to proactively provide access to the necessary raw material supplies (corn grain and sugar cane) at market pricing. These facilities are in Nebraska (U.S.) and in the Sao Paulo region of...
Castillo, Ernst, Lerch, Winchester

Brazil, respectively. Partnership discussions for woody biomass supply, in the Pacific Northwestern region of the United States, are currently in progress. This material is expected to be available in Washington State, and in the form of mill residue (but also land clearing debris and forest thinnings). Sugar supply from the dry mill is expected to be typical of that currently used to supply fuel-ethanol fermentations, while the Brazilian facility will supply molasses and cane juice at standard cane industry concentrations. In addition to raw material economics, your team will need to consider carefully the advantages, disadvantages, potential obstacles, and restrictions for each sugar supply option when making its selection; e.g., the sugar-cane crushing season in Brazil is 8-9 months long. Current market pricing is to be expected for all raw materials, utilities, and product, regardless of location.

A key point of the Directors’ interest involves the potential similarities and differences between facilities using woody biomass compared to molasses and cane juice, and sugar liberated from corn grain, including but not limited to, capital investment, overall process sustainability, and profitability. Your business director has determined that the process facilities and equipment should produce at a 400 MMlb per year capacity, using the technology documented in the patents, patent applications, and references listed below as an initial basis. Your para-xylene product must meet the minimum industry purity and quality standards for polymer intermediate grade material, as the expected end use is in bio-PET production. Given the recent volatility of petroleum markets and pricing, your marketing organization is unsure if this material will be able to command any premium above market pricing. Therefore, your business director believes sensitivity analyses are necessary to understand the potential exposure to market fluctuations, and any benefit that a market premium could provide.

This technology has potential use in the U. S. Corn Belt, where water is an extremely limited resource and a large area of concern for any potential plant site. Therefore, your plant and process design will need to use the minimum amount of water necessary for the technology, with the goal of being a zero-discharge plant (meaning that all process water is recycled within the plant). The current benchmark for total water use in a fuel-ethanol plant is about 3 gal/gal of product, and you should strive to meet or exceed this benchmark, regardless of raw biomass source.

Your plant design should be as environmentally friendly as possible, and satisfy the required state and federal emissions legislation. It is expected that the facility will include emission-control equipment as a part of the process design. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. Your plant design must be controllable and safe to operate. As the process technology integration and design team, you will participate in the start-up and will have to live with any of your poor design decisions.

Undoubtedly, you will need additional data beyond that given here and listed in the references below. Cite any literature data used. If required, make reasonable assumptions, state them, and identify whether your design or economics are sensitive to the assumptions you have made.

References

Virent BioForming® technology white paper,
U. S. Patent 8,017,818; Synthesis of Liquid Fuels and Chemicals from Oxygenated Hydro-Carbons; Cortright, R. D., et al; September 13, 2011.


U. S. Forestry Service has information available for woody biomass at: 


Appendix B: Sample Calculations

SC-000: Molasses Storage Requirements

The basic requirements for molasses storage are as follows: 1) molasses must be supplied at 1.245 Mlb/h, 2) there must be enough storage capacity to last three months, or 2208 h without replenishment, and 3) no one tank can exceed 20,000,000 gal. Additionally, given that the capacity should be within a “reasonable” range, the residence time is the key (least specified) variable of design. Vessel prices are estimated according to PPDP Table 22.32, with adjustments for the CE index change, $C_E$. The residence time is specified at six days, to permit active usage of five tanks at a time with once monthly deliveries.

Equations

$$V = \frac{Fr}{\rho_{mot}u}; C = C_E \times 265V^{0.51} \text{ (CS spherical, 0-30psig)}$$

Example

$$C = \frac{680}{500} \times 265 \left(\frac{\{1245000+144\}}{11.75+0.76}\right)^{0.51} = $1,906,822
The crystallizer must remove 2,293,914.1 BTU per hour in order to chill the mixed xylenes to -22 °F from 60°F. Additionally, the crystallizer requires 69.347 BTU per pound p-xylene to account for the latent heat of crystallization, and with 50,321.7 pounds per hour p-xylene product. This means 3,489,658.93 BTU per hour is required to crystallize the p-xylene. Therefore a total of 5,783,573.03 BTU per hour of refrigeration is used by the crystallizer unit.

At a cost of $10.867 per million BTU of heat removed for -90°F refrigerant, the total crystallization utilities are $62.85 per hour, or about $500,000 per year.
SC-700: Combustion Energy Availability

The amount of energy available from combustion is estimated from the flow rates and enthalpies of combustion of the major by-product species. Although there are many more hydrocarbon species in the process output, the light alkanes alone provide enough energy to cover the steam utility requirements. Therefore, this brief calculation (results tabulated in Figure 23) lends confidence to the notion that no outside steam would be necessary during normal operation.

Equations

\[ \dot{Q} = m \Delta H_{comb} \]

Figure 23

<table>
<thead>
<tr>
<th>By-Product</th>
<th>lbmol/h</th>
<th>lb/lbmol</th>
<th>Btu/lb</th>
<th>Btu/h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propane</td>
<td>639</td>
<td>44</td>
<td>21,700</td>
<td>611,503,830</td>
</tr>
<tr>
<td>Butane</td>
<td>45</td>
<td>58</td>
<td>20,900</td>
<td>54,661,860</td>
</tr>
<tr>
<td>Pentane</td>
<td>221</td>
<td>72</td>
<td>19,497</td>
<td>310,882,590</td>
</tr>
</tbody>
</table>

Total Energy Available: 977,048,280
SC-701: Sizing and Pricing for Heating Fluid Storage Vessels

The amount of heating fluid required is directly related to the net duty and the storage vessel residence. Net duties (Q) are calculated from ASPEN – these in turn are converted to mass flow rates via latent heat information (ΔH). The residence time (τ) for a storage vessel is a key determinant of how much fluid is required to be purchased up front. τ are chosen from recommendations or from the literature specifications. Capacity utilization (u) was taken at a conservative 70% for these units. Vessel prices are estimated according to PPDP Table 22.32, with adjustments for materials (F_M) according to PPDP p.580. The CE index change is accounted for by the multiplicative factor, C_E. Equations for all cases and an example calculation for Dowtherm A (ST-700), are shown below.

**Equations**

\[ V = \left( \frac{\dot{Q}}{\Delta H_v} \right) \tau \; ; \; C_P = 265 V^{0.51} \; \text{(CS cone roof)}; \; C_P = 47 V^{0.78} \; \text{(CS spherical, 30-200 psig)}; \; C = F_M C_P C_E \]

**Example**

\[ Q = 532 \; \text{MBtu/h}, \; \Delta H_v(700^\circ F) = 102 \; \text{Btu/lb}, \; \tau = 0.1 \; \text{h}, \; u = 70\%, \; P = 94 \; \text{psig}, \; \text{low-alloy} \]

\[ C_P = 47 \times \left( \frac{532 \times 10^6}{102} \right)^{0.1} = 441,074 \rightarrow C = 1.2 \times 441,074 \times \left( \frac{680}{500} \right) = 719,833. \]

SC-702: Pricing of Fired Heaters

Fired heaters are priced using Table 22.32 of PPDP and the desired heat duties, Q. The equations for all cases and an example for the molten salt heater are provided below. One source of concern is that the specified duties for the Dowtherm A and the steam boiler significantly exceed the specified range for the given equations. Prices were adjusted for the chemical engineering index and the material chosen.

**Equations**
Castillo, Ernst, Lerch, Winchester

\[ C_p = 12.32Q^{0.64} \text{ (molten salt); } C_p = 12.74Q^{0.65} \text{ (Dowtherm A); } C_p = 0.367Q^{0.77} \text{ (CS reboiler, P <20 atm); } C = F_M C_p C_E \]

Example

\[ Q = 62 \text{ MBtu/h, molten salt, stainless steel} \]

\[ C_p = 12.32(62 \times 10^6)^{0.64} = 1,196,028 \rightarrow C = 2.0 \times 1,196,028 \times \left( \frac{680}{500} \right) = 3,253,196. \]

**SC-U00: Heating Fluid Requirements and Costs**

Heat duties from ASPEN (Q) and materials information from the supplier (P, ΔHvap)

Appendix D provides the necessary information for these calculations, given a specified or assumed residence time (τ).

Equations

\[ m = \dot{m} \tau, \dot{m} = \frac{\dot{Q}}{\Delta H_{vap}} \text{ (condensing), } \dot{m} = \frac{\dot{Q}}{c \Delta T} \text{ (simple), } C = \hat{P} m \]

Example

\[ Q = 532 \text{ MBtu/h, condensing, } \Delta H_{vap} (700^9 F) = 101\text{Btu/lb, } \tau = 0.10 \text{ h, } \hat{P} = \$7.13/lb \]

\[ m = \frac{532 \times 10^6}{101} \times 0.10 = 532,000 \text{ lb } \rightarrow C = 7.13 \times 532,000 = 3,793,160. \]

**SC-U01: Utility Savings Calculations**

Utilities savings were calculated in two steps: 1) baseline utility requirements and 2) calculation of differential savings from substitution. From ASPEN, unit heat duties and temperatures are used to specify what utility is necessary, and how much. Pricing for baseline requirements is done using Table 23.1 in PPDP. Given the baseline, appropriate substitutes are sought from the process excess production, by-products, or integration opportunities. The substitutes are also priced according to Table 23.1. After annualizing, the difference in cost between baseline and substitute is the savings. An example is shown for steam, but an analogous procedure was followed for cooling and boiler feed water. Results for steam are shown in Figure 24.
Equations

\[ \dot{m} = \frac{Q}{\Delta H_{vap}} \text{ (condensing)} \quad C = \dot{m} \hat{P} \]

Example: RB-500

Given \( Q = 75.4 \text{ MBtu/h}, T = 296^\circ F \); Found \( P^s = 126 \text{ psig} \) (X-Eng Tables), \( \Delta H_{vap} \) (296\(^\circ F\)) \( =875 \text{ Btu/lb} \); Assumed \( \hat{P} = 4.80/1000 \text{ lb} \) (Table 23.1, PPDP)

\[ \dot{m} = \frac{75.4 \times 10^6}{875} = 86,174 \text{ lb/h} \rightarrow C = 4.80 \times 8.6174 \times 7920 = 3,134,780/\text{yr}. \]

Substituting boiler feed water: \( \hat{P}_{sub} = 1.80/1000 \text{ gal} \). Ignoring density changes as function of temperature, \( V = \frac{\dot{m}}{\rho} = \frac{8.6174}{8.32} \times 7920 = 82,000 \text{ kgal/yr} \rightarrow C = 1.80 \times 82,000 = $147,600 \)

Savings: $3.13M - $0.15M = $2.99M/yr

Figure 24

<table>
<thead>
<tr>
<th>Unit</th>
<th>Duty (Btu/h)</th>
<th>Temp (F)</th>
<th>Cond Temp (F)</th>
<th>Steam Pres (psig)</th>
<th>Utility Alternative (psig)</th>
<th>( \Delta H_{vap} ) (Btu/lb)</th>
<th>Amount (lb/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RB-500</td>
<td>75,402,272</td>
<td>296</td>
<td>341</td>
<td>126</td>
<td>150</td>
<td>875</td>
<td>86,174</td>
</tr>
<tr>
<td>RB-501</td>
<td>44,513,177</td>
<td>332</td>
<td>377</td>
<td>213</td>
<td>450</td>
<td>839</td>
<td>53,087</td>
</tr>
<tr>
<td>RB-502</td>
<td>146,774,702</td>
<td>239</td>
<td>284</td>
<td>52</td>
<td>50</td>
<td>922</td>
<td>159,192</td>
</tr>
<tr>
<td>RB-503</td>
<td>16,543,353</td>
<td>176</td>
<td>221</td>
<td>17</td>
<td>50</td>
<td>965</td>
<td>17,143</td>
</tr>
<tr>
<td>HX-301</td>
<td>32,323,000</td>
<td>360</td>
<td>405</td>
<td>260</td>
<td>450</td>
<td>822</td>
<td>39,327</td>
</tr>
<tr>
<td>WC-500</td>
<td>16,543,353</td>
<td>176</td>
<td>221</td>
<td>17</td>
<td>50</td>
<td>965</td>
<td>17,143</td>
</tr>
</tbody>
</table>

SC-C00

WHSV = mass of reactant fed per hour / mass catalyst = 13.5/7 \approx 1.93 \text{ hr}^{-1}

Mass of catalyst needed = 625000*453.6/1.93 = 147,000,000 grams of catalyst

Price of catalyst = 12/16 \times 1.47E8 \text{ price of } H_4SiO_4 \text{ per gram} + 1/16 \times 1.47E8 \text{ price of } Na_2AlO_2 \text{ per gram} + 3/16 \times 1.47E8 \text{ price of } (NH_4)_2SiF_6 \text{ per gram} = $2.49 \text{ million} \times 0.25 = $0.62 \text{ million}

Mass of deactivated catalyst per hour = 13.29 \times 1818.58 = 24,169 grams.
Yearly price = \((12/16 \times 24,169 \times \text{price of } H_4SiO_4 \text{ per gram} + 1/16 \times 24,169 \times \text{price of } Na_2AlO_2 \text{ per gram} + 3/16 \times 24,169 \times \text{price of } (NH_4)_2SiF_6 \text{ per gram}) \times 24 \times 365 = 3.52 \text{ million} \times 0.25 = 0.88 \text{ million}

**SC-C01**

“VHSV” = 300/40 = 7.5

\[ \text{SUF} = 17378.7 \times 28.3 / 0.04 / 7.5 = 1640368.8 \]

Toluene scale up = 300 \times \text{SUF} = 492.11 \text{ million ml}

Ruthenium (III) Acetylacetonate scale up = 2.907 \times \text{SUF} = 4.77 \text{ million grams}

\[ \text{Al}_2\text{O}_3 \text{ scale up} = 73 \times \text{SUF} = 119.75 \text{ million grams} \]

Price = Toluene scale up \times \text{Toluene density} \times \text{Toluene price} + Ruthenium (III) Acetyl Acetonate scale up \times \text{Ruthenium (III) Acetyl Acetonate price} + \text{Al}_2\text{O}_3 \text{ scale up} \times \text{Al}_2\text{O}_3 \text{ price} = 229.7 \text{ million} \times 0.25 = 57.4 \text{ million}

Ruthenium (III) Acetyl Acetonate wt% = 101/398 = 0.254

Mass of Ru in Ruthenium (III) Acetyl Acetonate scale up = Ruthenium (III) Acetyl Acetonate scale up \times 0.254 = 1.21 \text{ million grams}

Mass of catalyst needed = Mass of Ru in Ruthenium (III) Acetyl Acetonate scale up / 0.05 = 24.2 \text{ million grams}

Price of catalyst = price of similar catalyst \times \text{mass of catalyst needed} = 47.5 \text{ million} \times 0.25 = 11.9 \text{ million}

**SC-C02**

Mass of catalyst needed = 175,659 \times 453.6 / 1.8 = 44.27 \text{ million grams}

Number of batches needed = 44.27 \text{ million} / 19.875 = 2.46 \text{ million}

Price of catalyst = (Rhodium (III) Nitrate price \times Rhodium (III) Nitrate batch mass + Perrhenic acid price \times Perrhenic acid batch mass + Cerium (III) Nitrate price \times Cerium (III) Nitrate batch mass) \times 2.46 \text{ million} = 686 \text{ million}

Number batches needed = 44.27 \text{ million} / 13.28 = 3.33 \text{ million}

Price of catalyst = (Rhodium market price \times Rhodium batch mass + Rhenium market price \times Rhenium batch mass + Cerium market price \times Cerium batch mass + Titanium market price *
Titanium batch mass + Activated Carbon market price * Activated Carbon batch mass) * 3.33 million = $240.9 million * 0.25 = $60.2 million

**SC-C03**

Mass of catalyst needed = 530,125*453.6/1.93 = 120.2 million grams of catalyst

Price of catalyst = 30/31 * 120.2 million * price of H₄SiO₄ per gram + 1/31 * 120.2 million * price of Na₂AlO₂ per gram = $2.41 million *0.25 = $0.60 million

Mass of deactivated catalyst per hour = 13.29 * 2910 = 38,674 grams

Yearly price = (30/31 * 38,674 * price of H₄SiO₄ per gram + 1/31 * 38,674 * price of Na₂AlO₂ per gram) * 24 * 365 = $6.80 million * 0.25 = $1.70 million

**SC-C04**

WHSV = 12 (ml fed per hour in patent) * 0.8669 (density of toluene) / 2 (mass of catalyst in patent) = 5.2 hr⁻¹

Mass of catalyst needed = 144,783*453.6/1.93 = 12.6 million grams of catalyst

Price of catalyst = 70/71 * 12.6 million * price of H₄SiO₄ per gram + 1/71 * 12.6 million * price of Na₂AlO₂ per gram = $0.25 million *0.25 = $0.06 million

Mass of deactivated catalyst per hour = 13.29 * 1571.33 = 38,674 grams

Yearly price = (70/71 * 38,674 * price of H₄SiO₄ per gram + 1/71 * 38,674 * price of Na₂AlO₂ per gram) * 24 * 365 = $3.67 million * 0.25 = $0.92 million
DC-500 Concentration Profile

DC-500 Composition Profile

- p-xylene
- toluene
- benzene
- isopropylbenzene
- pentane
- hexane
### DC-500 Real Tray Efficiency Calculations

<table>
<thead>
<tr>
<th>Stage</th>
<th>K for p-xylene</th>
<th>K for toluene</th>
<th>Relative volatility</th>
<th>Viscosity liquid from (cP)</th>
<th>Efficiency</th>
<th>Real Trays</th>
<th>Real Tray</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.30</td>
<td>0.74</td>
<td>2.49</td>
<td>0.25</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>condenser</td>
</tr>
<tr>
<td>2</td>
<td>0.37</td>
<td>0.90</td>
<td>2.41</td>
<td>0.25</td>
<td>0.56</td>
<td>1.79</td>
<td>2.79</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.40</td>
<td>0.95</td>
<td>2.38</td>
<td>0.24</td>
<td>0.56</td>
<td>1.78</td>
<td>4.57</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.42</td>
<td>0.99</td>
<td>2.36</td>
<td>0.24</td>
<td>0.56</td>
<td>1.77</td>
<td>6.35</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.45</td>
<td>1.05</td>
<td>2.33</td>
<td>0.24</td>
<td>0.57</td>
<td>1.77</td>
<td>8.11</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.50</td>
<td>1.14</td>
<td>2.29</td>
<td>0.24</td>
<td>0.57</td>
<td>1.75</td>
<td>9.86</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.57</td>
<td>1.28</td>
<td>2.24</td>
<td>0.24</td>
<td>0.57</td>
<td>1.74</td>
<td>11.61</td>
<td>feed above</td>
</tr>
<tr>
<td>8</td>
<td>0.69</td>
<td>1.50</td>
<td>2.16</td>
<td>0.23</td>
<td>0.58</td>
<td>1.72</td>
<td>13.32</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.80</td>
<td>1.68</td>
<td>2.11</td>
<td>0.23</td>
<td>0.59</td>
<td>1.70</td>
<td>15.02</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.89</td>
<td>1.83</td>
<td>2.06</td>
<td>0.23</td>
<td>0.59</td>
<td>1.69</td>
<td>16.71</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.95</td>
<td>1.94</td>
<td>2.04</td>
<td>0.22</td>
<td>0.60</td>
<td>1.68</td>
<td>18.38</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1.00</td>
<td>2.02</td>
<td>2.02</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>20.06</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>1.03</td>
<td>2.07</td>
<td>2.01</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>21.73</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1.05</td>
<td>2.11</td>
<td>2.01</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>23.40</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>1.07</td>
<td>2.16</td>
<td>2.01</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>25.07</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>1.10</td>
<td>2.21</td>
<td>2.01</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>26.74</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>1.14</td>
<td>2.30</td>
<td>2.01</td>
<td>0.22</td>
<td>0.60</td>
<td>1.67</td>
<td>28.41</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1.22</td>
<td>2.45</td>
<td>2.02</td>
<td>0.23</td>
<td>1.00</td>
<td>1.00</td>
<td>29.41</td>
<td>reboiler</td>
</tr>
</tbody>
</table>
DC-501 McCabe Thiele Analysis
DC-502 McCabe Thiele Analysis
TRALSEP1 McCabe-Thiele Analysis (benzene/toluene)
SC-600: Sizing of HX-600

Section XII: Appendices

\[ \text{HX-600} \]

**Sizing of HX-600**

\[ \text{Q} = 62 \text{ MBtu/h} \]

\[ \text{AT}_{\text{m}} = \frac{\Delta T_{\text{m}}}{\ln \frac{0.719}{0.312}} = 378.6 \text{ °F} \]

\[ U = \frac{\text{Q}}{\text{AT}_{\text{m}}} = 189100 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F}} \right) \]

**EQUATION 1:**

\[ U \text{ is estimated from Table 18.5 in PPDP: } U < 200 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F} \cdot \text{ft}^2} \right) \text{ for water-organic exchange systems.} \]

**Estimation Method:**

- For exchanger sizes of 4 ft, \( U > 150 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F} \cdot \text{ft}^2} \right) \)
- For exchanger sizes of 4 ft, \( U < 500 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F} \cdot \text{ft}^2} \right) \)

**Rough conservative estimate:**

\[ \frac{1}{\text{AT}_{\text{m}}} = 2.0 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F} \cdot \text{ft}^2} \right) \]

So, the required heat exchange area is about 9500 ft².

**Cost Calculation:**

\[ C_B = \exp(11.908 + 0.879 \ln((9500) + 0.9005 \ln(9500))^2) = 896,700 \left( \frac{\text{Btu}}{\text{h} \cdot \text{°F}} \right) \text{ (PPDP 22.37)} \]

- Floating head

\[ C_C = \left( \frac{\text{Fm}}{\text{Ff}} \right)^{0.67} = 4.07 \]

- Stainless/stainless due to \( T = 1100^\circ \text{F} \)

\[ F_C = 20 \text{ ft tubes} \]

\[ F_P = 0.9805 + 0.018 \left( \frac{150}{100} \right) + 0.0017 \left( \frac{150}{100} \right)^2 = 1.01 \]

\[ P = 150 \text{ psig} \]

**CEH**

\[ \text{CEH} = 680 \text{ (extrapolation), so } \frac{C_P}{C_E} = \frac{\text{CE}}{C_C} = 898,450 \left( \frac{\text{Btu}}{\text{h}} \right) \]

\[ \text{Cost} = 96,700 \left( \frac{\text{Btu}}{\text{h}} \right) \times (0.07)(1.10)(1.01) \]

\[ = 398,450 \]

\[ = 541,700 \]
SYNTHESIS OF LIQUID FUELS AND CHEMICALS FROM OXYGENATED HYDROCARBONS

Inventors: Randy D. Cortright, Madison, WI (US); Paul G. Blomme, Oregon, WI (US)

Appl. No.: 13/157,247
Filed: Jan. 9, 2011

Publication Classification

Int. Cl.
C07C 9/00
C07C 1/207

U.S. Cl. 585/16; 585/240

Abstract

Processes and reactor systems are provided for the conversion of oxygenated hydrocarbons to hydrocarbons, ketones and alcohols useful as liquid fuels, such as gasoline, jet fuel or diesel fuel, and industrial chemicals. The process involves the conversion of mono-oxygenated hydrocarbons to aromatics and gasoline range hydrocarbons where the oxygenated hydrocarbons are derived from biomass.

Related U.S. Application Data

Continuation of application No. 12/044,837, filed on Mar. 7, 2008.

Provisional application No. 60/385,475, filed on Nov. 5, 2007, provisional application No 60/385,500, filed on Nov. 5, 2007, provisional application No. 60/390,573, filed on Mar. 8, 2007.
preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing air at 400°C.

Example 51

[0270] The same procedure used for preparing the catalyst of Example 50 was followed with the exception that the target rhenium loading was 1.8%.

Example 52

[0271] An 80:1 SiO₂:Al₂O₃ ratio ZSM-5 zeolite (Zeolyst International, CBV 8014) was mixed with a 1:1 molar ratio of ZnO and Al₂O₃ powders so that the ZnO and Al₂O₃ (Dispal 18N4-80, Sasol North America, Houston, Tex.) combined comprised 30 weight % of the total solids. Dilute nitric acid was added at a level of 2 weight % HNO₃ to the combined ZnO and Al₂O₃. The dough consistency was adjusted with water addition to form a workable dough suitable for extrusion and the mixture was extruded using a laboratory scale extruder. The extrudates were dried overnight under vacuum at 100°C and subsequently calcined at 600°C under flowing air.

Example 53

[0272] An aqueous solution of gallium nitrate was added to the material of Example 52, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen, using an incipient wetness technique to target a gallium loading of 1.2 weight %. The preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing hydrogen at 400°C.

Example 54

[0273] An aqueous solution of nickel nitrate was added to the material of Example 52, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen, using an incipient wetness technique to target a nickel loading of 1.0 weight %. The preparation was dried overnight in a vacuum oven and subsequently calcined in a stream of flowing hydrogen at 400°C.

Example 55

[0274] The catalyst systems referenced in Examples 6, 46, 48, 49, 51, 53, and 54 were investigated for the conversion of glycerol, sorbitol, sucrose, and xylose to hydrocarbons using the reactor configuration described in Example 2. The studies were conducted using two 21.2 mm internal diameter stainless steel tube reactors shown in Example 4, with an analysis completed as described in Example 5. Tungstated zirconia (NorPro-Saint Gobain, product code SZS1143, with particle sizes restricted to those that were maintained on a 60 mesh screen after passing through an 18 mesh screen) was placed on top of the condensation catalyst installed in the second reactor to provide a zone for vaporization of the first reactor effluent prior to entering the condensation catalyst.

[0275] Table 13 shows the results of these investigations. For Experiment NN (38% Sucrose+7% Xylose), a stream of hydrogen with a targeted flow rate equal to 3 times the moles of sucrose plus 1.5 times the moles of xylose was combined with the feed prior to entering the reactor. The other experiments were conducted without externally supplied hydrogen. Heaters external to the reactor, shown in FIG. 9, as 10a, 10b, 10c, 10d, 23a, 23b, 23c, and 23d, were used to maintain the reactor wall temperatures, as indicated in Table 13. The hydrocarbon products of these studies, disclosed in Table 13, were grouped into a C₅⁺ fraction, which are predominately present in the gas phase at ambient temperature and pressure, and a C₄⁺ fraction, which are generally suitable for incorporation into liquid fuels. The results show that a variety of sugars and polyhydric alcohols may be readily converted to C₅⁺ hydrocarbons by the processes described herein. The products contained mainly paraffins and aromatic constituents. The breakdown of paraffins and aromatics within this sample is shown in FIG. 17.

### Table 13

| Conversion of Sugars and Polyhydric Alcohols to C₅⁺ Hydrocarbons |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Experiment      | NN              | OO              | PP              | QQ              |
| Hydrogenation   | Example 6       | Example 48      | Example 49      | Example 50      |
| API/Oxidation   | Example 6       | Example 51      | Example 51      | Example 50      |
| Condensation    | Example 6       | Example 48      | Example 49      | Example 50      |
| Catalyst Loadings | Example 6       | Example 48      | Example 49      | Example 50      |
| Hydrogenation   | grams           | grams           | grams           | grams           |
| API/Oxidation   | grams           | grams           | grams           | grams           |
| Tungstated Zirconia | grams          | grams           | grams           | grams           |
| Condensation    | grams           | grams           | grams           | grams           |
| Heater Block Temperature Ranges, Inlet of Catalyst Bed - Outlet of Catalyst Bed |
| Hydrogenation   | °C             | 100-150         | 245-256         | 245-265         |
| API/Oxidation   | °C             | 250-270         | 355-365         | 355-375         |
| Tungstated Zirconia | °C             | 375-375         | 375-375         | 375-375         |
| Condensation    | °C             | 350-350         | 350-350         | 350-350         |
| Pressure        | psig            | 625             | 625             | 625             |
| 1st Reactor Outlet | psig           | 625             | 625             | 625             |
| 2nd Reactor Outlet | psig           | 625             | 625             | 625             |
| Feed            | psig            | 625             | 625             | 625             |
| Sucrose + 7% Xylose | None            | Glycerol        | Glycerol        | Glycerol        |

249
<table>
<thead>
<tr>
<th>Experiment</th>
<th>NN</th>
<th>OO</th>
<th>PP</th>
<th>QQ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen production WHSV</td>
<td>1.6</td>
<td>1.9</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>C\textsubscript{4} Alkanes</td>
<td>21.2</td>
<td>26.9</td>
<td>8.1</td>
<td>13.0</td>
</tr>
<tr>
<td>C\textsubscript{4} Olefins</td>
<td>1.1</td>
<td>1.4</td>
<td>1.3</td>
<td>5.2</td>
</tr>
<tr>
<td>Total C\textsubscript{4} Hydrocarbons</td>
<td>22.3</td>
<td>28.3</td>
<td>9.4</td>
<td>18.1</td>
</tr>
<tr>
<td>C\textsubscript{5} Paraffins</td>
<td>20.0</td>
<td>7.9</td>
<td>9.5</td>
<td>11.3</td>
</tr>
<tr>
<td>C\textsubscript{5} Olefins</td>
<td>0.8</td>
<td>1.9</td>
<td>1.2</td>
<td>7.8</td>
</tr>
<tr>
<td>Naphthenes</td>
<td>1.9</td>
<td>1.4</td>
<td>1.6</td>
<td>1.2</td>
</tr>
<tr>
<td>Aromatics</td>
<td>25.0</td>
<td>17.8</td>
<td>48.4</td>
<td>22.3</td>
</tr>
<tr>
<td>Other C\textsubscript{5} Hydrocarbons</td>
<td>0.0</td>
<td>1.1</td>
<td>0.2</td>
<td>3.4</td>
</tr>
<tr>
<td>Total C\textsubscript{5} Hydrocarbons</td>
<td>47.7</td>
<td>30.1</td>
<td>61.0</td>
<td>46.1</td>
</tr>
</tbody>
</table>
FIG 17
United States Patent [19]
Black et al.

[54] METHOD OF SEPARATING LIGNOCELLULOSIC MATERIAL INTO LIGNIN, CELLULOSE AND DISSOLVED SUGARS

[75] Inventors: Stuart K. Black, Denver; Bonnie R. Hames, Westminster; Michele D. Myers, Dacono, all of Colo.

[73] Assignee: Midwest Research Institute, Kansas City, Mo.

[21] Appl. No.: 348,469

[51] Int. Cl.6 ........................................ D21C 3/20
[52] U.S. Cl. ........................................ 162/16; 162/72; 162/77; 127/37
[58] Field of Search ................................ 162/72, 76, 77, 162/29, 16; 127/37

[56] References Cited
U.S. PATENT DOCUMENTS
1,594,389 8/1926 Thelker
1,888,025 11/1933 Beat
2,024,689 12/1935 Groomsidge


2,037,009 4/1936 Arokovys
2,042,705 6/1936 Dreyfas
3,545,104 6/1971 Rievert .............................. 162/77
3,932,307 1/1976 Pogansky
3,951,734 4/1976 DeHaas .............................. 162/72
4,552,105 5/1985 Sinner
4,594,130 6/1986 Chang

FOREIGN PATENT DOCUMENTS

Primary Examiner—Steven Alvo
Attorneys, Agent, or Firm—Edna M. O'Connor, Ruth Eure

ABSTRACT
A method for separating lignocellulosic material into (a) lignin, (b) cellulose, and (c) hemicellulose and dissolved sugars. Wood or herbaceous biomass is digested at elevated temperature in a single-phase mixture of alcohol, water and a water-immiscible organic solvent (e.g., a ketone). After digestion, the amount of water or organic solvent is adjusted so that there is phase separation. The lignin is present in the organic solvent, the cellulose is present in a solid pulp phase, and the aqueous phase includes hemicellulose and any dissolved sugars.

8 Claims, No Drawings
1. METHOD OF SEPARATING LIGNOCELLULOSIC MATERIAL INTO LIGNIN, CELLULASE AND DISSOLVED SUGARS

CONTRACTUAL ORIGIN OF THE INVENTION

The United States Government has rights in this invention under Contract No. DE-AC36-83CH10933 between the United States Department of Energy and the National Renewable Energy Laboratory, a Division of the Midwest Research Institute.

BACKGROUND OF THE INVENTION

1. Field of the Invention

The present invention relates to methods and techniques for the fractionation of wood and herbaceous biomass. More particularly, this invention relates to methods and techniques for separating wood and biomass into three major components for further processing.

2. Description of the Prior Art

Pulping processes have previously been used for separating cellulose from lignin and other components of lignocellulosic materials. For example, various types of inorganic chemicals in water have been used to modify lignin to render it water soluble. Those processes, however, present problems in recovering or destroying the inorganic chemicals. Other processes have been proposed using organic solvents for dissolving the lignin from the lignocellulosic material. Such processes can be expensive because of the cost of solvent recovery. Still other processes have involved combinations of acids and alcohols with water. However, the presence of excess water can be detrimental to the process, and use of high concentrations of acid require costly recovery systems.

U.S. Pat. No. 2,037,001 (Aronovsky) describes an extraction process involving a two component aqueous alcoholic liquor. Lignin is separated from the aqueous stream by cooling the pulping liquid to ambient temperature following digestion and allowing the liquor to phase separate. The dissolved lignin is carried with the alcohol while any dissolved sugars remain in the aqueous liquor. The purity of lignin products isolated from processes using alcohol is not as high as is desired. An impure lignin isolated from alcohol requires extensive and expensive purification. Also, use of cooling temperatures for phase separation of the liquor could lead to re-deposition of lignin on the fibers.

U.S. Pat. No. 1,594,389 (Thellier) deals with the removal of extractives from flax and similar plants using a water/hydrocarbon mixture. This extraction would not remove any of the structural components of the flax nor would it result in the fractionation of the material due to the low concentration of the hydrocarbon which would remain soluble in the water.

U.S. Pat. No. 1,888,025 (Bent) describes a process in which wood or lignocellulosic material is extracted with aqueous organic solvents followed by the recovery of relatively hydrophobic extractives into an immiscible hydrophobic solvent. The patent deals with the removal of resin from wood—essentially an extractive in pine wood—with an aqueous alcoholic solvent followed by a liquid/liquid extraction of the resin from the solvent rather than the separation of biomass into structural polymer components.

U.S. Pat. No. 2,024,689 (Groombridge) refers to the use of mixtures of organic compounds with water for the separation of cellulose from the noncellulosic material in lignocellulosic feedstocks. However, there is no description of the use of a water-immiscible organic compound, water and a water-soluble organic compound to effect this separation.

U.S. Pat. No. 2,042,705 (Dreyfus) describes a process very similar to Groombridge, above, with the addition of water to the solvate mixture. There is no description of the separation of the pulping liquor into a lignin-rich component and a hemimcellulose-rich component.

U.S. Pat. No. 3,932,207 (Pogorzelsky) describes a process in which, prior to cooking, fragments of lignocellulosic material are impregnated with a solution of a lignin-solubilizing reagent in an organic solvent with a boiling point higher than the cooking temperature. Then the impregnated material is immersed in a liquid which is immiscible with the solvent of the solution.

U.S. Pat. No. 4,520,105 (Sinac) describes a process involving a chemical pretreatment with a mixture of water and lower alcohols or acetone, after which the residue is separated and then treated with a similar solvent mixture at elevated temperature. However, alcohol or acetone mixtures with water cannot be separated into two phases. Also, separation of the lignin from dissolved sugars would require further processing through extensive washing.

U.S. Pat. No. 4,594,130 (Chang) describes a cooking process, in the absence of oxygen, at elevated temperatures with a neutral or acidic mixture of alcohol and water containing a magnesium, calcium or barium salt as a catalyzer. The catalyst is for the purpose of aiding retention of the hemicellulose in the cellulose case.

European Patent Application 86205606.5 (Biodyne) describes a process for digesting lignocellulosic material with an ester, an organic lignin solvent and water. The lignin solvents are either an organic acid or alcohol or terephthalic acid, and it is miscible in both the ester and the water. Cooling of the liquor apparently results in some phase separation, but a centrifuge is also required.

There has not heretofore been described an efficient process involving the use of a single phase cooking liquor which can be readily separated into two liquid phases when desired.

SUMMARY OF THE INVENTION

It is an object of the invention to provide a process for separating wood and herbaceous biomass into its three major components for further processing.

It is an object of the invention to provide a convenient and efficient process for separating lignocellulosic material into lignin, cellulose, hemicellulose and sugars thereof. It is another object of the invention to provide a process for separating lignocellulosic material into its three major components using either a batch process or a continuous process.

It is yet another object of the invention to provide a very pure lignin stream in a process for fractionating lignocellulosic material.

It is still another object of this invention to provide a cellulose stream free of re-precipitated lignin in a process for fractionating lignocellulosic material.

Additional objects, advantages, and novel features of the invention shall be set forth in part in the description that follows and in part will become apparent to those skilled in the art upon examination of the following or may be learned by the practice of the invention. The objects and the advantages of the invention may be realized and attained by means of the instrumentalities and in combinations particularly pointed out in the appended claims.
Section XII: Appendices

5,730,837

To achieve the foregoing and other objects and in accordance with the purpose of the present invention, as embodied and broadly described herein, the improved methods may comprise separating lignocellulosic material into lignin, (b) cellulose, and (c) hemicellulose and sugars. In one embodiment the method comprises:

(a) digesting the lignocellulosic material in a single phase mixture of alcohol, water and a water-immiscible organic solvent selected from the group consisting of ketones;

(b) adjusting the amount of water in said mixture to cause phase separation;

(c) separating said mixture into first, second and third phases; wherein said first phase comprises lignin and said organic solvent, said second phase comprises solid cellulose cake, and said third phase is an aqueous alcoholic mixture and comprises hemicellulose and dissolved sugars.

The methods and techniques provided by this invention enable wood or herbaceous biomass to be fractionated very efficiently in a single phase, after which the pulping mixture can be separated into separate phases wherein the lignin is present in a homogeneous organic phase, the hemicellulose and sugars are present in the aqueous phase, and cellulose is present as a solid colloidal cake. The organic phase can be separated, and the lignin can be isolated by evaporation of the organic solvent. The isolated lignin is substantially free of sugars.

The separate components of the wood and herbaceous biomass can be used for further desired processing. For example, the cellulose can be used for making paper and paperboard products or ethanol. It can also be used for making cellulose derivatives such as cellulose ethers. The lignin can be used as a feedstock for phenolics, enhanced oil recovery surfactants, or fuel additives. The hemicellulose can be used making ethanol or other chemicals.

Other advantages of the methods of this invention will be apparent from the following detailed description.

DETAILED DESCRIPTION OF THE INVENTION

The improved methods of this invention involve placing the lignocellulosic material (e.g., wood or herbaceous biomass) in a suitable reactor, after which a mixture of solvents and water  are added. It is necessary to obtain a single phase mixture. A water-insoluble or water-immiscible organic solvent is used which is a ketone. A water-soluble or miscible alcohol and water are also used. Preferably the ketone is an aliphatic ketone having at least 4 carbon atoms (and may have as many as 10 carbon atoms). The alcohol preferably has less than about 4 carbon atoms to assure that it will be water-miscible.

Useful aliphatic ketones include, for example, methyl ethyl ketone, methyl isopropyl ketone, methyl propyl ketone, methyl butyl ketone, methyl isobutyl ketone, methyl isoamyl ketone, diethyl ketone, ethyl isopropyl ketone, ethyl propyl ketone, and ethyl isobutyl ketone. Useful alcohols include methanol, ethanol, propanol, isopropanol and butanol.

Typically the ketone is present in the solvent system in an amount of about 7 to 65% by weight, and water is present in an amount of about 10 to 65% by weight. The alcohol is typically present in an amount of about 25 to 35% by weight. The weight ratio of ketone to water is preferably in the range of about 1:9 to 6:5:1, so long as a single phase of digesting liquid is obtained.

Typically, the weight ratio of liquor to wood or biomass is at least about 4:1 and could be much greater if desired, e.g., 8:1 or 10:1.

The digestion is preferably carried out at an elevated temperature. Typically the digestion mixture is heated in the reactor to a temperature in the range of about 100° to 220° C. Some types of biomass can be digested more quickly than other types. If desired, a concept called severity may be used to determine the length of time required to obtain complete digestion of a particular biomass. The term severity involves use of an empirically derived equation relating time at temperature and the temperature above a base temperature at which reaction does not occur. The concept and the equation are explained in Organosolv Pretreatment for Enzymatic Hydrolysis of Poplar. 2. Catalyst Effects and the Combined Severity Parameter, H. L. Chum, D. K. Johnston, and S. K. Black, I & EC Research, 1990, 29, 156-162. Incorporated herein by reference.

After the digestion has been completed, the single phase can be easily converted into two liquid phases upon the addition of either water or water-immiscible solvent. The two phases have very little cross-contamination of components from one phase into the other. The lignin stream is very pure and is easily isolated by evaporation of the organic solvent which is water-immiscible. The cellulose stream obtained is free of re-precipitated lignin because the lignin and other dissolved materials remain in solution at all temperatures of the reaction. The lignin and hemicellulose are dissolved away from the wood chips leaving an insoluble colloidal cake.

An acid catalyst is added to reduce the reaction temperature from about 200° C for uncatalyzed cook to 140° C for a catalyzed cook. It also reduces the amount of time required. The catalysts used are mineral acids such as sulfuric or phosphoric acid. Nitric acid may also be used but it is not as effective. The amount of catalyst used varies with the feedstock but is generally in the range of 0.025M to 0.2M (0.2 to 2 wt % of the liquor used).

The processes of this invention are useful for fractionating all types of lignocellulosic material into separate components. For example, the processes may be used in connection with wood and herbaceous derived materials such as sugar cane bagasse, switch grass, and legumes.

EXAMPLE 1

Poplar wood chips (15.7 g oven-dried equivalent) were charged into a 200 ml batch reactor. A single phase pulping liquor composed of 24% water, 44% methyl isobutyl ketone (MIBK) and 32% ethanol with a 0.05 M H₂SO₄ catalyst was added in a ratio of 10 parts liquor to 1 part wood. The reactor was placed in a preheated heating block. The reactor was held at 140° C for 56 minutes after a 34 minute heat-up time. Severity of the reaction was 4.3. The resulting pulp was fiberized in a Waring blender and washed with fresh neutral liquor. The oven-dried equivalent yield of pulp was 64%. Kappa number for this pulp was measured at 72.

Water was added to the liquor in a ratio of 1.3 parts water to 1 part liquor to cause phase separation of the insoluble MIBK component. Lignin was isolated from the MIBK phase by evaporation with a yield of 18%. Klassen lignin analysis of this lignin gave a 88% purity. Dissolved sugars composed mostly of hemicellulose were contained in the combined alcohol-aqueous fraction in a 18% yield based on the wood charged.

EXAMPLE 2

Under the same conditions as above, 14.4 g of oven-dried equivalent poplar was charged into a batch reactor. A
EXAMPLE 3

Aspen chips (193 g, oven-dried equivalent) were charged into a 1.7 liter percolation reactor. The reactor was filled with a MIBK/ethanol/water mixture containing 16% MIBK, 34% ethanol and 50% water containing 0.025M \( \text{H}_2\text{SO}_4 \). The reactor was heated to 140° C. over 34 minutes without flow of solvent. When the pulping temperature was reached, pulping solvent of the same composition was pumped through the chip bed at a flow rate of 28 ml/min, for 36 minutes. The chips were then washed in the reactor with neutral solvent at the same flow rate for 60 minutes without heating. Total severity for the reaction was 4.27. The reactor was drained, the chips fiberized and the lignin separated as described above. The pulp yield was 52% with a Kappa of 28. Lignin was isolated in a 17% yield. Hemicellulose yield was 31%.

EXAMPLE 4

Poplar chips from underbarked logs (189 g, oven-dried equivalent) were pulped under the same conditions as example 3 except for a 0.1 M \( \text{H}_2\text{SO}_4 \) catalyst concentration. Severity for this run was 4.27. The pulp yield was 45% with a Kappa of 4.2. Lignin was isolated in a 22% yield at a purity of 93%. Hemicellulose yield was 33%.

EXAMPLE 5

Depithed sugar cane bagasse (72 g, oven-dried equivalent) was pulped under the same conditions as example 4. The solvent mixture used was the same as that of example 1. Severity was 4.23. The yield of pulp was 49% with a Kappa of 3. The yield of lignin was 32%. Yield of hemicellulose was 19%.

The foregoing is considered as illustrative only of the principles of the invention. Further, since numerous modifications and changes will readily occur to those skilled in the art, it is not desired to limit the invention to the exact construction and operation shown and described. Accordingly, all suitable modifications and equivalents may be resorted to falling within the scope of the invention as defined by the claims which follow. The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

What is claimed is:

1. A method for separating lignocellulosic material into lignin, cellulose, and dissolved sugars composed mostly of hemicellulose and sugars, the method comprising the steps of:

(a) digesting lignocellulosic material in a single phase mixture of an alcohol, water and a water-immiscible ketone having at least 4 carbon atoms to solubilize lignin and hemicellulose and leave a cellulose solid phase; said water being present in said single phase mixture in an amount of about 10 to 65 percent by weight, and said water-immiscible ketone being present in an amount of about 7 to about 65% by weight;

(b) adjusting the amount of water in said single liquid phase mixture to cause phase separation into two liquid phases of a lignin water-immiscible ketone stream and a stream of dissolved sugars composed mostly of hemicellulose; and

(c) separating said mixture into first, second and third phases; wherein said first phase is a liquid and comprises high purity lignin by evaporating water-immiscible ketone; said second phase comprises high purity cellulose in a solid phase; and said third phase is an aqueous and comprises hemicellulose and dissolved sugars.

2. A method in accordance with claim 1, wherein said digesting is carried out at a temperature in the range of about 135° C. to 220° C.

3. A method in accordance with claim 1, wherein said ketone is selected from the group consisting of methyl isobutyl ketone, methyl isopropyl ketone methyl isovalyl ketone.

4. A method in accordance with claim 1, wherein said alcohol has 1-4 carbon atoms.

5. A method in accordance with claim 1, wherein said single phase mixture further comprises an acid catalyst.

6. A method in accordance with claim 5, wherein said acid catalyst comprises a mineral acid which is present in an amount about 0.2 to 2% by weight.

7. A method in accordance with claim 6, wherein said catalyst is selected from the group consisting of sulfuric acid and phosphoric acid.

8. A method for separating lignocellulosic material into lignin, cellulose, and dissolved sugars composed mostly of hemicellulose and sugars, the method comprising the steps of:

(a) digesting lignocellulosic material in a single phase mixture of an alcohol, water and a water-immiscible ketone having at least 4 carbon atoms to solubilize lignin and hemicellulose and leave a cellulose solid phase; said water being present in said single phase mixture in an amount of about 10 to 65 percent by weight, and said water-immiscible ketone being present in an amount of about 7 to about 65% by weight;

(b) adjusting the amount of said ketone in said single liquid phase mixture to cause phase separation into two liquid phases of a lignin water-immiscible ketone stream and a stream of dissolved sugars composed mostly of hemicellulose; and

(c) separating said mixture into first, second and third phases; wherein said first phase is a liquid and comprises high purity lignin by evaporating water-immiscible ketone said second phase comprises high purity cellulose in a solid phase; and said third phase is an aqueous alcohol mixture and comprises hemicellulose and dissolved sugars.
Manufacture of high purity benzene and para-rich xylenes by combining aromatization and selective disproportionation of impure toluene

Inventors: Gerald J. Nacamuli, Mill Valley; Robert A. Innes, San Rafael; Arnold J. Glown, Walnut Creek, all of CA (US)

Assignee: Chevron Corporation, San Ramon, CA (US)

Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 0 days.

Related U.S. Application Data

Continuation-in-part of application No. 08/273,933, filed on Jul. 12, 1994, now abandoned, which is a continuation of an application No. 07/984,248, filed on Sep. 13, 1993, now abandoned, which is a continuation of an application No. 07/852,412, filed on Sep. 28, 1992, now abandoned, which is a continuation of an application No. 07/790,987, filed on Jul. 11, 1992, now abandoned.

Int. Cl. 7; C07C 6/00; C07C 15/04; C07C 15/08

U.S. Cl. 585/475; 585/312; 585/322

Field of Search 585/475; 585/312; 585/322

References Cited

U.S. PATENT DOCUMENTS

3,957,624 * 5/1976 Bornacchi et al. 585/475
4,046,219 * 4/1977 Kaufing 585/475
4,052,476 * 10/1977 Movienet 585/475
4,069,919 * 1/1978 Hartter 585/475
4,097,549 * 6/1978 Han et al. 585/475
4,160,788 * 7/1979 Young 585/475
4,360,002 * 1/1983 Chu 585/475
4,501,403 * 1/1990 Chu 585/475
4,862,257 * 10/1989 Ashby et al. 585/475

* cited by examiner

Primary Examiner—Elizabeth D. Wood
Attorney, Agent, or Firm—Thomas G. D.C. St. John
Charles W. Stewart

A process is set forth for reacting impure toluene to obtain benzene, toluene and a para-rich xylene stream, which are substantially free of close-boiling non-aromatics. The impure toluene comprises at least 70 wt% toluene and between about 0.2 wt% and about 5 wt% close-boiling non-aromatics. The process may also include aromatizing a naphtha over a non-acidic catalyst. The impure toluene from the aromatization step is passed over an acidic intermediate pore zeolite to produce a para-rich xylene stream and chemically pure benzene.

19 Claims, 3 Drawing Sheets
The present invention will be more clearly understood by reference to the following examples.

**EXAMPLE 1**

**Comparison Example with Non-selectivated Catalyst:**

Debottleneck reformate prepared by reforming of a full boiling-range naphtha feedstock over a catalyst comprising platinum on alumina and was distilled to obtain light and heavy fractions. The heavy reformate was further distilled to a 30% cut point. The overhead product of the second distillation, comprising about 92 wt% toluene and about 8 wt% nonaromatics, was vaporized, blended with hydrogen, and passed through a tubular fixed-bed reactor charged with acidic but not selectivated ZSM-5 catalyst. The reaction was carried out at 1000°F (538°C), 150 psig, and 5.7 liquid toluene feed weight hourly space velocity (WHSV). The added hydrogen/toluene molar ratio was about 3:1.

Feed and product analyses were obtained by capillary gas-liquid chromatography after nine hours on stream, as shown in Table 1. The gas chromatograph was equipped with a flame ionization detector and a polar column that eluted nonaromatics before aromatics.

<table>
<thead>
<tr>
<th>Components</th>
<th>Feed Area %</th>
<th>Product Area %</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nonaromatics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1-C5</td>
<td>0.004</td>
<td>5.536</td>
<td>5.532</td>
</tr>
<tr>
<td>toluene</td>
<td>0.032</td>
<td>0</td>
<td>-0.002</td>
</tr>
<tr>
<td>x-benzene</td>
<td>0.010</td>
<td>0</td>
<td>-0.000</td>
</tr>
<tr>
<td>C6-C7</td>
<td>0.092</td>
<td>0</td>
<td>-0.092</td>
</tr>
<tr>
<td>nonaromatics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n-xylene</td>
<td>0.334</td>
<td>0</td>
<td>-0.334</td>
</tr>
<tr>
<td>C7-C8</td>
<td>2.044</td>
<td>0</td>
<td>-2.035</td>
</tr>
<tr>
<td>nonaromatics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>m-xylene</td>
<td>0.933</td>
<td>0</td>
<td>-0.933</td>
</tr>
<tr>
<td>C8+C9</td>
<td>1.423</td>
<td>0.116</td>
<td>-1.307</td>
</tr>
<tr>
<td>nonaromatics</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C9 + aromatics</td>
<td>0.431</td>
<td>0.027</td>
<td>-0.404</td>
</tr>
</tbody>
</table>

**Aromatization Followed by Selectiviated Para-xylene Production**

A C1 to C6 naphtha was aromatized over a non-acidic platinum L-zeolite catalyst by being fed via line 10 (refer to FIG. 1) to an aromatization unit 12. The aromatization was run to maximize yield of benzene whereby the resulting liquid product contained only a small amount of unreacted C6 to C9 naphtha components. The C9 + aromatic product stream was collected. It was then taken, as represented by line 14 and was separated in a distillation column 16 into a benzene-rich fraction (removed as represented by line 18) and a C9 + aromatic bottoms fraction, both having close-boiling nonaromatics. Most of the unreacted paraffins, olefins and naphthenes were found in the benzene overhead fraction rather than the toluene and heavy aromatics C9 + aromatic fraction after distillation. As a result, the feed (bottoms fraction) to the toluene disproportionation step which followed contained about 0.4 wt% close boiling non-aromatics. The benzene fraction was sent as represented by line 37 aromatics extraction unit 56.

The conditions during the aromatization process were as follows:

Naphtha WISV=1.0, feed molar ratio H2/naphtha=5:0, temperature=980°F, pressure=70 psig.

The C6 bottoms fraction, along with some of the hydrogen from the aromatization unit 12 introduced as represented by line 20, was fed via line 22 to a disproportionation zone 24 wherein it was contacted with a selectivated intermediate pore size zeolite catalyst whereby para-xylene was selectively produced and close boiling non-aromatics were converted to materials which boil generally outside of the benzene and xylenes ranges. Excess hydrogen was removed from the aromatization unit 12 via line 25 and light hydrocarbons were removed via line 27. The toluene fraction was reacted over an acidic, large crystallite size (0.5-2.0) HZSM-5 (Silica to alumina ratio of 70:1) catalyst, which had previously been selectivated by passing toluene and nitrogen over the catalyst at 1100°F and 150 psig for 27 hours. 12 ml of toluene, feed and 75°C to 75°F of hydrogen were passed over 2 grams of catalyst at 850°F and 150 psig. Table 2 shows the analysis of the toluene fraction of the aromatization product and of the product of the selectivated conversion of toluene to benzene and para-xylene.

<table>
<thead>
<tr>
<th>Components, Wt %</th>
<th>Feed</th>
<th>Product</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light Ends</td>
<td>0.00</td>
<td>0.71</td>
<td>0.71</td>
</tr>
<tr>
<td>C9 non-aromatics</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.11</td>
<td>10.35</td>
<td>10.24</td>
</tr>
<tr>
<td>C7 non-aromatics</td>
<td>0.11</td>
<td>0.02</td>
<td>-0.09</td>
</tr>
<tr>
<td>Toluene</td>
<td>65.79</td>
<td>65.36</td>
<td>-0.42</td>
</tr>
<tr>
<td>C9 + aromatic</td>
<td>34.21</td>
<td>34.65</td>
<td>+0.44</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>2.41</td>
<td>1.51</td>
<td>-0.90</td>
</tr>
<tr>
<td>Heavy aromatics</td>
<td>7.02</td>
<td>3.46</td>
<td>-3.56</td>
</tr>
</tbody>
</table>

**TABLE 2**

<table>
<thead>
<tr>
<th>Components, Wt %</th>
<th>Feed</th>
<th>Product</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light Ends</td>
<td>0.00</td>
<td>0.71</td>
<td>0.71</td>
</tr>
<tr>
<td>C9 non-aromatics</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.11</td>
<td>10.35</td>
<td>10.24</td>
</tr>
<tr>
<td>C7 non-aromatics</td>
<td>0.11</td>
<td>0.02</td>
<td>-0.09</td>
</tr>
<tr>
<td>Toluene</td>
<td>65.79</td>
<td>65.36</td>
<td>-0.42</td>
</tr>
<tr>
<td>C9 + aromatic</td>
<td>34.21</td>
<td>34.65</td>
<td>+0.44</td>
</tr>
<tr>
<td>p-Xylene</td>
<td>2.41</td>
<td>1.51</td>
<td>-0.90</td>
</tr>
<tr>
<td>Heavy aromatics</td>
<td>7.02</td>
<td>3.46</td>
<td>-3.56</td>
</tr>
</tbody>
</table>

Total 99.99 100.00 0.01

**Conditions**

<table>
<thead>
<tr>
<th>Component</th>
<th>Selectivated Large Crystallite HZSM-5</th>
</tr>
</thead>
</table>

The analyses show that the toluene disproportionated to make benzene and xylenes, while nonaromatic impurities in the same boiling range were substantially eliminated by cracking to form light ends. Para-xylene comprised 24 wt% of the xylenes produced.

This example demonstrates the elimination of close boiling nonaromatics and the preparation of chemically pure benzene and xylene using a non-para-selective catalyst whereby close boiling of the xylene fraction was para-xylene.
TABLE 2—continued

<table>
<thead>
<tr>
<th>Composition</th>
<th>Flow</th>
<th>Product</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst Weight = 2.0 Gms</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Final Feed Rate = 52 m/hr</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature = 836°F</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure = 150 psig</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td>74%</td>
<td>p-Xylene</td>
<td>100%</td>
</tr>
<tr>
<td>m-Xylene + o-Xylene + Xylene</td>
<td>25%</td>
<td>m-Xylene + o-Xylene + Xylene</td>
<td>100%</td>
</tr>
</tbody>
</table>

Better than 80% of the close boiling non-aromatic material in the toluene fraction was converted to light or heavy ends in the toluene disproportionation reactor leaving only 0.2% C₈ non-aromatics in the final product relative to 10.35 wt % benzene and 0.60 wt % C₈ aromatics relative to 14.31 wt % xylene. Thus the benzene stream has a purity of 99.8 wt %. About 90% of the ethylbenzene and a proportion of the ortho-xylene and heavy aromatics in the original feed were converted yielding even more benzene and para-xylene. The para-xylene proportion of the xylene fraction was 68.3 wt %.

Hydrogen and light hydrocarbons from the disproportionation zone 24 are recycled via line 29 to the aromatization unit 12. The rest of the product from the disproportionation zone 24 is conducted via line 26 to distillation column 28 where it is distilled to provide a bottom fraction having C₈ aromatics and being enriched in para-xylene which is removed via line 30 and an overhead fraction containing C₅ and C₆ aromatics. The C₈ aromatics stream is sent to a para-xylene plant for the recovery of para-xylene and the aromatization of ortho- and meta-xylene to para-xylene, operating costs in the para-xylene plant are significantly reduced because the toluene disproportionation unit produces a xylene stream which 1) is substantially free of non-aromatics, 2) is rich in the para-xylene isomer and 3) contains a reduced amount of ethylbenzene.

The C₅-C₆ aromatics fraction is conducted via line 32 to a further distillation column 34 where it is further distilled to provide toluene for sending via line 31 to the disproportionation zone 24 (or for recovery as a chemically pure product) and to provide high pure benzene as an overhead. This benzene is combined via line 33 with the high purity benzene obtained from the aromatics extraction unit 36. The benzene product is chemically pure and the xylene product is substantially free of non-aromatics. The xylene product is enriched in para-xylene. The para-xylene proportion of the xylene fraction is 60 to 80 wt %.

This example demonstrates the production of high purity benzene and a para-enriched xylene stream from a C₅-C₆ naphtha. The process comprises aromatization of a C₅-C₆ naphtha followed by para-selective disproportionation of impure toluene.

EXAMPLE 3

Process Starting with C₅-C₆ Naphtha

A C₅ naphtha is fed via line 38 (see FIG. 2) to an aromatization reactor 40 along with hydrogen gas which may be fed via line 42. The aromatics and close boiling non-aromatics contained in the product from the reactor are fed via line 44 to a disproportionation zone 46 containing an acidic intermediate pore size noble catalyst which has been selectivized for para-xylene production. Hydrogen is separated from the product of the disproportionation zone 46 in flash drum 48 and removed via line 47. All or a portion of the hydrogen can be recycled, for example, via compressor 49, to the aromatization reactor 40 via line 42. The remainder of the product is fed via line 50 to a stabilizer column 52 wherein light hydrocarbons are stripped off and removed via line 51. The bottoms fraction from the stabilizer column is fed via line 54 to a benzene recovery column 56 wherein toluene is removed as the overhead via line 64 and sent to the disproportionation zone 46 (or recovered as a chemically pure product). The bottom fraction from the benzene recovery column contains chemical grade C₆ aromatics enriched in para-xylene. The para-xylene proportion of the xylene fraction is 60 to 80 wt %.

This example demonstrates high para-xylene yield with the product being of chemical grade quality starting with a C₅ naphtha.

FIG. 3 illustrates this example which is similar to the embodiment of FIG. 1. A C₅-C₆ full boiling range naphtha is fed to aromatization unit 12 via line 10. Hydrogen and light hydrocarbons are removed via lines 25 and 27. The remainder of the aromatization product is fed via line 14 to distillation column 16. The overhead from column 16 contains benzene and lighter components. It is fed to benzene extractor 36. The raffinate from extractor 36 is cycled to the aromatization unit 12 via line 37. A chemically pure benzene product is removed via line 57.

The bottoms fraction from column 16 is delivered via line 22 to a distillation column 60. C₅ aromatics are removed via line 60 via line 62 and can be used as a heavy gasoline blending stock. The C₆-C₆ overhead from column 60 is led via line 64 to a further distillation column 66.

Distillation column 66 separates the C₆-C₆ overhead from column 60 into a C₆ product which is removed via line 30 and into a C₅-C₆ overhead which is further separated in distillation column 34 into chemically pure benzene and into toluene which is sent to disproportionation unit 24 via line 31 (or is recovered as pure xylene). The chemically pure benzene from unit 34 is combined with the chemically pure benzene from unit 34. The toluene stream is disproportionated to yield chemically pure benzene, toluene and para-rich-xylene. The toluene disproportionation product then proceeds to the distillation train via line 26 and high purity benzene, toluene and C₆ aromatics are removed as described above.

The above example demonstrates the wide applicability of the process of the present invention for the production of para-xylene enriched xylene along with high purity benzene from full boiling range naphthas and from toluene-rich feedstocks which can be prepared from such naphthas.

INDUSTRIAL APPLICABILITY

The present invention provides the capability of synthesizing chemical grade benzene and para-xylene enriched
(54) Title: CATALYSTS AND METHODS FOR REFORMING OXYGENATED COMPOUNDS

(57) Abstract: Disclosed are catalysts and methods that can reform aqueous solutions of oxygenated compounds such as ethylene glycol, glycerol, sugar alcohols, and sugars to generate products such as hydrogen and alkanes. In some embodiments, aqueous solutions containing at least 20 wt% of the oxygenated compounds can be reformed over a catalyst comprising a Group VIII transition metal and a Group VIIB transition metal, preferably supported on an activated carbon-supported catalyst. In other embodiments, catalysts are provided for the production of hydrogen or alkanes at reaction temperatures less than 300°C.
Example 30

[0118] Functionalized carbon surfaces were modified by impregnation of metal oxides prior to impregnation of catalyst precursors. Titanium n-butoxide, 1.95g, was diluted to 12mL with anhydrous isopropanol. This solution was added by incipient wetting to air oxidation functionalized carbon (see Example 26 above), 10g. The wetted carbon was dried under vacuum at 100°C overnight.

Example 31 (RhReCe catalyst, 5% wt. Rh, 1:1:1 molar ratio Re:Rh:Ce)

[0119] Rhodium(III) Nitrate, 3.86g, Perrhenic Acid, 1.64g, and Cerium(III) Nitrate hexahydrate, 2.21g, were dissolved in enough DI water to make 12mL of solution. This solution was added by incipient wetting to Titania modified carbon from Example 30, and then dried under vacuum at 100°C overnight.

Example 32

[0120] The catalysts of Examples 25 through 31 were pretreated under flowing hydrogen at 250°C, before the liquid feed containing oxygenated compounds were introduced to the catalyst at the desired reaction temperature. Table 5 shows the results of reforming the different solutions over these catalysts. When compared to the results for the conversion of higher concentrations of glycerol presented in Example 24, Table 5 shows that the combination of rhenium and Group VIII metals supported on activated carbon significantly enhances the activity for the reforming of higher concentrations of oxygenated compounds.
Table 7. Effect of Addition of Base to Feed on Activity and Selectivity for APR Catalysts.

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Catalyst</th>
<th>Ex.</th>
<th>Base</th>
<th>Wt % M</th>
<th>Molar Ratios (Re:Rh:Ce or Re:Pt)</th>
<th>WHSV (hr⁻¹)ᵃ</th>
<th>Conversion to Gas (%)</th>
<th>Gas Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>30% Sorbitol</td>
<td>RhReCe</td>
<td>NAᵇ</td>
<td>none</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>70%</td>
<td>47% 12% 40%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>RhReCe</td>
<td>b</td>
<td>0.5% NaOH</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.7</td>
<td>71%</td>
<td>53% 8% 39%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>RhReCe</td>
<td>b</td>
<td>1.25% NaOH</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>78%</td>
<td>57% 8% 37%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>RhReCe</td>
<td>b</td>
<td>1.5% NaOH</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>75%</td>
<td>56% 8% 34%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>RhReCe</td>
<td>b</td>
<td>1.65% NaOH</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>73%</td>
<td>56% 8% 34%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>PtRe</td>
<td>28</td>
<td>none</td>
<td>5% Pt</td>
<td>2.5:1</td>
<td>2.2</td>
<td>57%</td>
<td>36% 12% 47%</td>
</tr>
<tr>
<td>30% Sorbitol</td>
<td>PtRe</td>
<td>28</td>
<td>2.5% KOH</td>
<td>5% Pt</td>
<td>2.5:1</td>
<td>2.2</td>
<td>64%</td>
<td>55% 7% 36%</td>
</tr>
<tr>
<td>50% Sorbitol</td>
<td>RhReCe</td>
<td>31</td>
<td>none</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>81%</td>
<td>49% 19% 35%</td>
</tr>
<tr>
<td>50% Sorbitol</td>
<td>RhReCe</td>
<td>31</td>
<td>1.65% NaOH</td>
<td>5% Rh</td>
<td>1:1:1</td>
<td>1.8</td>
<td>75%</td>
<td>57% 12% 33%</td>
</tr>
</tbody>
</table>

ᵃ Weight hour space velocities (WHSV) are based on feed rate of oxygenated substrate.
ᵇ preparation of this catalyst (on H₂O₂ vanadium modified carbon) was not described in any example, but the procedure was similar to example 34.

Example 37

[0125] A 3 wt% platinum catalyst supported on activated carbon was prepared according to the general method of Example 1. An aqueous solution, approximately 9.5mL, containing 0.75g of dihydrogen hexachloroplatinate (IV) hexahydrate (Alfa Aesar, 39.85% Pt) and 1.22g of perhenic acid solution (Alfa Aesar, 79.18% HReO₄) was added to 10.0g peroxide functionalized carbon (Calgon UU, sieved to 60-120 mesh functionalized using the method of Example 20). The mixture was dried at 100°C under vacuum.

- 30 -
Appendix D: Materials

Dowtherm A Specifications

DOWTHERM A

Synthetic Organic Heat Transfer Fluid — Liquid and Vapor Phase Data

DOWTHERM A heat transfer fluid is a eutectic mixture of two very stable compounds, biphenyl (C_{12}H_{10}) and diphenyl oxide (C_{12}H_{10}O). These compounds have practically the same vapor pressures, so the mixture can be handled as if it were a single compound. DOWTHERM A fluid may be used in systems employing either liquid phase or vapor phase heating.

Recommended use temperature range:
Liquid phase: 15°C (60°F) to 400°C (750°F)
Vapor phase: 257°C (495°F) to 400°C (750°F)

Suitable applications: Indirect heat transfer

For health and safety information for this product, contact your Dow sales representative or call the number for your area on the second page of this sheet for a Material Safety Data Sheet (MSDS).

Typical Properties of DOWTHERM A Fluid

<table>
<thead>
<tr>
<th>Property</th>
<th>SI Units</th>
<th>English Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freeze Point</td>
<td>120°C</td>
<td>250°F</td>
</tr>
<tr>
<td>Atmospheric Boiling Point</td>
<td>257.1°C</td>
<td>495.8°F</td>
</tr>
<tr>
<td>Flash Point*</td>
<td>112°C</td>
<td>233°F</td>
</tr>
<tr>
<td>Fire Point*</td>
<td>118°C</td>
<td>246°F</td>
</tr>
<tr>
<td>Autoignition Temperature*</td>
<td>590°C</td>
<td>1102°F</td>
</tr>
<tr>
<td>Density @ 25°C (77°F)</td>
<td>1036 kg/m³</td>
<td>66.0 lb/ft³</td>
</tr>
<tr>
<td>Surface Tension in Air @ 20°C (68°F)</td>
<td>40.1 Dynes/cm</td>
<td>40.1 Dynes/cm</td>
</tr>
<tr>
<td></td>
<td>40°C (104°F)</td>
<td>37.6 Dynes/cm</td>
</tr>
<tr>
<td></td>
<td>60°C (140°F)</td>
<td>33.7 Dynes/cm</td>
</tr>
<tr>
<td>Estimated Critical Temperature</td>
<td>497°C</td>
<td>923°F</td>
</tr>
<tr>
<td>Estimated Critical Pressure</td>
<td>31.34 bar</td>
<td>30.93 atm</td>
</tr>
<tr>
<td>Estimated Critical Volume</td>
<td>3.17 l/kg</td>
<td>0.0508 ft³/lb</td>
</tr>
<tr>
<td>Average Molecular Weight</td>
<td>166.0</td>
<td></td>
</tr>
<tr>
<td>Heat of Combustion</td>
<td>36.053 kJ/kg</td>
<td>15,500 Btu/lb</td>
</tr>
</tbody>
</table>

*Not to be combined as specifications

Saturated Liquid Properties of DOWTHERM A Fluid (SI units)

<table>
<thead>
<tr>
<th>Temp. °C</th>
<th>Vapor Pressure psi</th>
<th>Viscosity m²/sec</th>
<th>Specific Heat °C/Btu/lb °F</th>
<th>Thermal Cond. W/m K</th>
<th>Density kg/m³</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.00</td>
<td>0.00</td>
<td>1.938</td>
<td>0.1995</td>
<td>1033.5</td>
</tr>
<tr>
<td>35</td>
<td>0.00</td>
<td>0.00</td>
<td>1.701</td>
<td>0.1315</td>
<td>1023.7</td>
</tr>
<tr>
<td>100</td>
<td>0.00</td>
<td>0.00</td>
<td>1.814</td>
<td>0.1201</td>
<td>990.7</td>
</tr>
<tr>
<td>155</td>
<td>0.00</td>
<td>0.00</td>
<td>1.954</td>
<td>0.1171</td>
<td>947.8</td>
</tr>
<tr>
<td>225</td>
<td>0.00</td>
<td>0.00</td>
<td>2.093</td>
<td>0.1091</td>
<td>902.2</td>
</tr>
<tr>
<td>255</td>
<td>0.00</td>
<td>0.00</td>
<td>2.231</td>
<td>0.1011</td>
<td>854.0</td>
</tr>
<tr>
<td>355</td>
<td>0.00</td>
<td>0.00</td>
<td>2.373</td>
<td>0.0931</td>
<td>801.3</td>
</tr>
<tr>
<td>405</td>
<td>0.00</td>
<td>0.00</td>
<td>2.527</td>
<td>0.0851</td>
<td>742.3</td>
</tr>
</tbody>
</table>

Saturated Liquid Properties of DOWTHERM A Fluid (English units)

<table>
<thead>
<tr>
<th>Temp. °F</th>
<th>Vapor Pressure psia</th>
<th>Viscosity cP</th>
<th>Specific Heat Btu/lb °F</th>
<th>Thermal Cond. W/m K</th>
<th>Density lb/ft³</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
<tr>
<td>200</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
<tr>
<td>300</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
<tr>
<td>400</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
<tr>
<td>500</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
<tr>
<td>600</td>
<td>0.00</td>
<td>4.911</td>
<td>2.073</td>
<td>0.0005</td>
<td>88.27</td>
</tr>
</tbody>
</table>

*Trademark of The Dow Chemical Company
DOWTHERM A
Synthetic Organic Heat Transfer Fluid

Saturated Vapor Properties of DOWTHERM A Fluid (SI Units)

<table>
<thead>
<tr>
<th>Temp. °C</th>
<th>Vapor Pressure bar</th>
<th>Liquid Enthalpy kJ/kg</th>
<th>Latent Heat kJ/kg</th>
<th>Vapor Density kg/m³</th>
<th>Vapor Enthalpy kJ/kg</th>
<th>Vapor Volume Conc. Wt/%</th>
<th>Z</th>
<th>Specific Heat (cP) J/g·K</th>
<th>Ratio of Specific Heats (cP/cV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.00</td>
<td>4.9</td>
<td>407.2</td>
<td>412.1</td>
<td>0.0044</td>
<td>0.0075</td>
<td>1.000</td>
<td>1.044</td>
<td>1.050</td>
</tr>
<tr>
<td>25</td>
<td>0.00</td>
<td>88.1</td>
<td>380.9</td>
<td>406.1</td>
<td>0.0040</td>
<td>0.0104</td>
<td>1.000</td>
<td>1.227</td>
<td>1.043</td>
</tr>
<tr>
<td>35</td>
<td>0.01</td>
<td>158.1</td>
<td>362.7</td>
<td>520.9</td>
<td>0.0041</td>
<td>0.0129</td>
<td>0.996</td>
<td>1.364</td>
<td>1.028</td>
</tr>
<tr>
<td>45</td>
<td>0.06</td>
<td>251.2</td>
<td>314.5</td>
<td>592.7</td>
<td>0.0083</td>
<td>0.0163</td>
<td>0.985</td>
<td>1.528</td>
<td>1.035</td>
</tr>
<tr>
<td>55</td>
<td>0.28</td>
<td>351.2</td>
<td>320.2</td>
<td>671.5</td>
<td>0.0090</td>
<td>0.0200</td>
<td>0.982</td>
<td>1.681</td>
<td>1.034</td>
</tr>
<tr>
<td>65</td>
<td>0.97</td>
<td>458.2</td>
<td>297.4</td>
<td>753.6</td>
<td>0.0101</td>
<td>0.0238</td>
<td>0.964</td>
<td>1.629</td>
<td>1.036</td>
</tr>
<tr>
<td>75</td>
<td>2.40</td>
<td>572.2</td>
<td>271.5</td>
<td>843.5</td>
<td>0.0110</td>
<td>0.0279</td>
<td>0.958</td>
<td>1.676</td>
<td>1.042</td>
</tr>
<tr>
<td>85</td>
<td>5.80</td>
<td>600.1</td>
<td>240.6</td>
<td>932.8</td>
<td>0.0212</td>
<td>0.0322</td>
<td>0.938</td>
<td>2.133</td>
<td>1.057</td>
</tr>
<tr>
<td>95</td>
<td>11.92</td>
<td>923.0</td>
<td>301.7</td>
<td>1033.7</td>
<td>0.1190</td>
<td>0.0382</td>
<td>0.740</td>
<td>2.932</td>
<td>1.064</td>
</tr>
</tbody>
</table>

Saturated Vapor Properties of DOWTHERM A Fluid (English Units)

<table>
<thead>
<tr>
<th>Temp. °F</th>
<th>Vapor Pressure psia</th>
<th>Liquid Enthalpy Btu/lb</th>
<th>Latent Heat Btu/lb</th>
<th>Vapor Density lb/ft³</th>
<th>Vapor Enthalpy Btu/lb</th>
<th>Vapor Volume Conc. Wt/%</th>
<th>Z</th>
<th>Specific Heat (cP) Btu/lb·°F</th>
<th>Ratio of Specific Heats (cP/cV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>30.00</td>
<td>26.2</td>
<td>167.3</td>
<td>193.5</td>
<td>0.0060</td>
<td>0.0055</td>
<td>1.000</td>
<td>0.276</td>
<td>1.045</td>
</tr>
<tr>
<td>60</td>
<td>56.4</td>
<td>103.0</td>
<td>148.0</td>
<td>251.1</td>
<td>0.0130</td>
<td>0.0079</td>
<td>0.996</td>
<td>0.361</td>
<td>1.035</td>
</tr>
<tr>
<td>70</td>
<td>200.0</td>
<td>131.1</td>
<td>142.0</td>
<td>273.1</td>
<td>0.0189</td>
<td>0.0106</td>
<td>0.992</td>
<td>0.335</td>
<td>1.031</td>
</tr>
<tr>
<td>80</td>
<td>3.28</td>
<td>160.0</td>
<td>148.8</td>
<td>296.3</td>
<td>0.0267</td>
<td>0.0120</td>
<td>0.977</td>
<td>0.400</td>
<td>1.024</td>
</tr>
<tr>
<td>90</td>
<td>12.25</td>
<td>191.4</td>
<td>142.2</td>
<td>320.5</td>
<td>0.2200</td>
<td>0.0135</td>
<td>0.950</td>
<td>0.433</td>
<td>1.035</td>
</tr>
<tr>
<td>100</td>
<td>31.7</td>
<td>233.5</td>
<td>132.1</td>
<td>346.4</td>
<td>0.403</td>
<td>0.0140</td>
<td>0.922</td>
<td>0.486</td>
<td>1.030</td>
</tr>
<tr>
<td>110</td>
<td>44.31</td>
<td>256.9</td>
<td>114.2</td>
<td>371.1</td>
<td>0.7289</td>
<td>0.0186</td>
<td>0.913</td>
<td>0.480</td>
<td>1.045</td>
</tr>
<tr>
<td>120</td>
<td>64.89</td>
<td>287.7</td>
<td>95.3</td>
<td>397.0</td>
<td>1.234</td>
<td>0.0212</td>
<td>0.973</td>
<td>0.595</td>
<td>1.055</td>
</tr>
<tr>
<td>130</td>
<td>122.7</td>
<td>327.9</td>
<td>95.0</td>
<td>422.9</td>
<td>2.045</td>
<td>0.0200</td>
<td>0.780</td>
<td>0.534</td>
<td>1.073</td>
</tr>
<tr>
<td>140</td>
<td>188.4</td>
<td>365.9</td>
<td>82.5</td>
<td>448.4</td>
<td>3.270</td>
<td>0.0219</td>
<td>0.714</td>
<td>0.571</td>
<td>1.108</td>
</tr>
</tbody>
</table>

For further information, call...

In the United States and Canada: 1-800-447-4359 · FAX: 1-989-832-1465
In Europe: +32 3 450 2240 · FAX: +32 3 450 2815
In the Pacific: +866 22 547 8731 · FAX: +886 22 713 0092
In other Global Areas: 1-989-932-1560 · FAX: 1-989-932-1465

www.dowtherm.com

Notices: The data, charts, and material presented by DOW are designed for your use to be correct. However, use or application of the data, charts, and material is at your own risk. The above information is subject to change without notice. It is provided for your use as a reference only. The products described in this document are not intended for use in or around nuclear facilities. DOW makes no representations, warranties, or certifications that their use will not violate any United States or foreign laws or regulations. DOW specifically disclaims any implied warranties of merchantability or fitness for a particular purpose. In the event that any implied warranty is not disclaimed in law, the duration of such warranty is limited to the duration of this warranty. No warranties exist. If your use of the products, charts, or data described herein is prohibited by law, this warranty shall not apply.

Published November 2001

Prepared in U.S.A. © Dow Chemical Company N.A./Pacific: Form No. 176-91483-1101-AMIS
Europe: CH133-087-E-1101

264
### Table 1 Parametric operating conditions for analyses

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power block type</td>
<td>Steam Rankine cycle</td>
</tr>
<tr>
<td>Power block capacity</td>
<td>55 MWe gross</td>
</tr>
<tr>
<td>Steam turbine inlet conditions:</td>
<td></td>
</tr>
<tr>
<td>Pressure Temperature</td>
<td>66 bar, 100 bar, nominally 400-500°C</td>
</tr>
<tr>
<td>Steam turbine cycle efficiency:</td>
<td>determined by GateCycle calculation, nominally 38.5-41.1% for these conditions.</td>
</tr>
<tr>
<td>Solar field outlet salt temperature:</td>
<td>Nominal Maximum</td>
</tr>
<tr>
<td></td>
<td>Maximum</td>
</tr>
<tr>
<td></td>
<td>450°C~500°C</td>
</tr>
<tr>
<td>Optical:</td>
<td>Overall optical efficiency 0.75</td>
</tr>
<tr>
<td>Performance runs:</td>
<td>Thermal storage capacity 6h</td>
</tr>
<tr>
<td>Annual Insolation</td>
<td>Barstow</td>
</tr>
<tr>
<td>Collector type</td>
<td>Generic SEGs type with advanced features</td>
</tr>
<tr>
<td>Receiver</td>
<td>Current Solel Receiver</td>
</tr>
<tr>
<td>Operating scenario</td>
<td>Solar only</td>
</tr>
</tbody>
</table>

### Table 2 Characteristics of the Nitrate Salts and Therminol VP-1

<table>
<thead>
<tr>
<th>Property</th>
<th>Solar Salt</th>
<th>Hitec</th>
<th>Hitec XL (Calcium Nitrate Salt)</th>
<th>LiNO₃ mixture</th>
<th>Therminol VP-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composition, %</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Diphenyl biphenyl oxide</td>
</tr>
<tr>
<td>NaNO₃</td>
<td>60</td>
<td>7</td>
<td>7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>KNO₃</td>
<td>40</td>
<td>53</td>
<td>45</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NaNO₂</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ca(NO₃)₂</td>
<td></td>
<td></td>
<td>48</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Freezing Point, °C</td>
<td>220</td>
<td>142</td>
<td>120</td>
<td>120</td>
<td>13</td>
</tr>
<tr>
<td>Upper Temperature, °C</td>
<td>600</td>
<td>535</td>
<td>500</td>
<td>550</td>
<td>400</td>
</tr>
<tr>
<td>Density @ 300°C, kg/m³</td>
<td>1899</td>
<td>1840</td>
<td>1992</td>
<td>815</td>
<td></td>
</tr>
<tr>
<td>Viscosity @ 300°C, cp</td>
<td>3.26</td>
<td>3.16</td>
<td>6.37</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Heat capacity @ 300°C, J/kg·K</td>
<td>1495</td>
<td>1560</td>
<td>1447</td>
<td>2319</td>
<td></td>
</tr>
</tbody>
</table>
Table 3  Effective Storage Fluid Cost

<table>
<thead>
<tr>
<th>Salt</th>
<th>Temperature Rise °C</th>
<th>Cost per Kg $/kg</th>
<th>Storage Cost $/kWh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hitec (a) [142°C]</td>
<td>200</td>
<td>0.93</td>
<td>10.7</td>
</tr>
<tr>
<td>Solar Salt (b) [220°C]</td>
<td>200</td>
<td>0.49</td>
<td>5.8</td>
</tr>
<tr>
<td>Calcium Nitrate</td>
<td>200</td>
<td>1.19</td>
<td>15.2</td>
</tr>
<tr>
<td>[HitecXL] (c) [120°C]</td>
<td>150</td>
<td>1.19</td>
<td>20.1</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>1.19</td>
<td>30.0</td>
</tr>
<tr>
<td>Therminol VP-1 (d)</td>
<td>100</td>
<td>2.2</td>
<td>57.5</td>
</tr>
</tbody>
</table>

a) 7.53 Na.K Nitrate, 40 Na Nitrite  
b) 60:40 Na.K Nitrate  
c) 42:15:43 Ca:Na.K Nitrate  
d) Diphenyl/biphenyl oxide
Material Safety Data Sheet
Sucrose MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sucrose
Catalog Codes: SLS4048, SLS3253, SLS1036
CAS#: 57-50-1
RTECS: WN6500000
TSCA: TSCA (b) Inventory: Sucrose
Cl#: Not available.
Synonym: beta-D-Fructofuranosyl-alpha-D-glucopyranoside
Chemical Name: Sucrose
Chemical Formula: C12H22O11

Contact Information:
ScienceLab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sucrose</td>
<td>57-50-1</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification

Potential Acute Health Effects: Slightly hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention if irritation occurs.
Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.
Auto-Ignition Temperature: Not available.
Flash Point: CLOSED CUP: Higher than 93.3°C (200°F).
Flammable Limits: Not available.
Products of Combustion: These products are carbon oxides (CO, CO₂).
Fire Hazards in Presence of Various Substances: Slightly flammable to flammable in presence of heat.
Fire Fighting Media and Instructions: SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.
Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.
Large Spill: Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions: Keep locked up. Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibilities such as oxidizing agents, acids.
Section XII: Appendices

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Safety glasses. Lab coat. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Personal Protection In Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 15 (mg/m³) from OSHA (PEL) [United States] Inhalation Total. TWA: 10 (mg/m³) from ACGIH (TLV) [United States] [1999] Inhalation Total. TWA: 10 (mg/m³) from NIOSH Inhalation Total. TWA: 5 (mg/m³) from NIOSH Inhalation Respirable. TWA: 5 (mg/m³) from OSHA (PEL) [United States] Inhalation Respirable.3 Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline granules solid.)
Odor: Characteristic Carmel to Odorless.
Taste: Sweet.
Molecular Weight: 342.3 g/mole
Color: White.
PH (1% soln/water): Not available.
Boiling Point: Not available.
Melting Point: 186°C (366.8°F)
Critical Temperature: Not available.
Specific Gravity: 1.587 (Water = 1)
Vapor Pressure: Not applicable.
Vapor Density: Not available.
Vapility: Not available.
Odor Threshold: Not available.
Water/Oil Dist. Coeff.: The product is more soluble in water; log(oil/water) = -3.7
Ionicity (In Water): Not available.
Dispersion Properties: See solubility in water, methanol.

Section 10: Stability and Reactivity Data
Stability: The product is stable.  
Instability Temperature: Not available.  
Conditions of Instability: Excess heat, incompatible materials  
Incompatibility with various substances: Reactive with oxidizing agents, acids.  
Corrosivity: Not available.  
Special Remarks on Reactivity: Reactive with sulfuric acid, nitric acid, and oxidizers.  
Special Remarks on Corrosivity: Not available.  
Polymerization: Will not occur.

### Section 11: Toxicological Information

**Routes of Entry:** Inhalation, ingestion.  
**Toxicity to Animals:** Acute oral toxicity (LD50): 29700 mg/kg [Rat].  
**Chronic Effects on Humans:**  
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast.  
**Other Toxic Effects on Humans:** Slightly hazardous in case of skin contact (irritant), of ingestion, of inhalation.  
**Special Remarks on Toxicity to Animals:** Not available.  
**Special Remarks on Chronic Effects on Humans:**  
No adverse reproductive affects have been found in humans. However at extremely high oral doses of 653,000 mg/kg given to rats during pregnancy showed some effects on newborn (growth, developmental anomalies of central nervous system). Passes through the placental barrier in human.  
**Special Remarks on other Toxic Effects on Humans:**  
Acute Potential Health Effects: Skin: May cause skin irritation. Low hazard for usual industrial handling. Eyes: Dust may cause mechanical irritation. Inhalation: Excessive inhalation may cause minor respiratory irritation. Ingestion: Ingestion of large amounts may cause gastrointestinal (digestive) tract irritation. Expected to be a low ingestion hazard. Chronic Potential Health Effects: no information.

### Section 12: Ecological Information

**Ecotoxicity:** Not available.  
**BOD5 and COD:** Not available.  
**Products of Biodegradation:**  
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.  
**Toxicity of the Products of Biodegradation:** The product itself and its products of degradation are not toxic.  
**Special Remarks on the Products of Biodegradation:** Not available.

### Section 13: Disposal Considerations

**Waste Disposal:**  
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

### Section 14: Transport Information
Section XII: Appendices

Section 15: Other Regulatory Information

Federal and State Regulations:
Rhode Island RTK hazardous substances; Sucrose Pennsylvania RTK: Sucrose Minnesota: Sucrose Massachusetts RTK: Sucrose Tennessee: Sucrose TSCA 8(b) Inventory: Sucrose

Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:
WHMIS (Canada): Not controlled under WHMIS (Canada).
DSCL (EEC):
This product is not classified according to the EU regulations. S24/25- Avoid contact with skin and eyes.

HMIS (U.S.A.):
- Health Hazard: 1
- Fire Hazard: 1
- Reactivity: 0
- Personal Protection: X

National Fire Protection Association (U.S.A.):
- Health: 1
- Flammability: 1
- Reactivity: 0
- Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Safety glasses.

Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/10/2005 08:28 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Water MSDS

Section 1: Chemical Product and Company Identification
Product Name: Water
Catalog Codes: SLW1063
CAS#: 7732-18-5
RTECS: ZC0110000
TSCA: TSCA 8(b) Inventory: Water
Cl#: Not available.
Synonym: Dihydrogen oxide
Chemical Name: Water
Chemical Formula: H2O
Contact Information:
          ScienceLab.com, Inc.
          14025 Smith Rd.
          Houston, Texas 77396
          US Sales: 1-800-901-7247
          International Sales: 1-281-441-4400
          Order Online: ScienceLab.com
          CHEMTREC (24HR Emergency Telephone), call:
          1-800-424-9300
          International CHEMTREC, call: 1-703-527-3887
          For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients
Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>7732-18-5</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification
Potential Acute Health Effects:

Potential Chronic Health Effects:

Section 4: First Aid Measures
Eye Contact: Not applicable.
Section XII: Appendices

Section 5: Fire and Explosion Data

<table>
<thead>
<tr>
<th>Flammability of the Product:</th>
<th>Non-flammable.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto-ignition Temperature:</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Flash Points:</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Flammable Limits:</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Products of Combustion:</td>
<td>Not available.</td>
</tr>
<tr>
<td>Fire Hazards in Presence of Various Substances:</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Explosion Hazards in Presence of Various Substances:</td>
<td>Not Applicable</td>
</tr>
<tr>
<td>Fire Fighting Media and Instructions:</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Special Remarks on Fire Hazards:</td>
<td>Not available.</td>
</tr>
<tr>
<td>Special Remarks on Explosion Hazards:</td>
<td>Not available.</td>
</tr>
</tbody>
</table>

Section 6: Accidental Release Measures

| Small Spill: | Mop up, or absorb with an inert dry material and place in an appropriate waste disposal container. |
| Large Spill: | Absorb with an inert material and put the spilled material in an appropriate waste disposal. |

Section 7: Handling and Storage

| Precautions: | No specific safety phrase has been found applicable for this product. |
| Storage:     | Not applicable. |

Section 8: Exposure Controls/Personal Protection

| Engineering Controls: | Not Applicable |
| Personal Protection:  | Safety glasses. Lab coat. |
| Personal Protection In Case of a Large Spill: | Not Applicable |
| Exposure Limits:      | Not available. |

Section 9: Physical and Chemical Properties

| Physical state and appearance: | Liquid. |
### Section 10: Stability and Reactivity Data

- **Stability:** The product is stable.
- **Instability Temperature:** Not available.
- **Conditions of Instability:** Not available.
- **Incompatibility with various substances:** Not available.
- **Corrosivity:** Not available.
- **Special Remarks on Reactivity:** Not available.
- **Special Remarks on Corrosivity:** Not available.
- **Polymerization:** Will not occur.

### Section 11: Toxicological Information

- **Routes of Entry:** Absorbed through skin. Eye contact.
- **Toxicity to Animals:**
  - **LD50:** [Rat] - Route: oral; Dose: > 90 ml/kg LC50: Not available.
  - **Chronic Effects on Humans:** Not available.
- **Other Toxic Effects on Humans:**
- **Special Remarks on Toxicity to Animals:** Not available.
Section XII: Appendices

Special Remarks on Chronic Effects on Humans: Not available.
Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information
Ecotoxicity: Not available.
BOD5 and COD: Not available.
Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The product itself and its products of degradation are not toxic.
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations
Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information
DOT Classification: Not a DOT controlled material (United States).
Identification: Not applicable.
Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information
Federal and State Regulations: TSCA 8(b) Inventory: Water
Other Regulations: EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.
Other Classifications:
WHMIS (Canada): Not controlled under WHMIS (Canada).
DSCL (EEC):
This product is not classified according to the EU regulations. Not applicable.
HMIS (U.S.A.):
Health Hazard: 0
Fire Hazard: 0
Reactivity: 0
Personal Protection: 3
National Fire Protection Association (U.S.A.):
Health: 0
Flammability: 0
Reactivity: 0
Specific hazard:
Protective Equipment:
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/10/2005 08:33 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Dextrose anhydrous MSDS

Section 1: Chemical Product and Company Identification
Product Name: Dextrose anhydrous
Catalog Codes: SLD3860, SLD4483
CAS#: 50-99-7
RTECS#: LZ5600000
TSCA: TSCA 8(b) Inventory: Dextrose anhydrous
Ctd: Not available.
Synonym: D-Glucose
Chemical Name: Not available.
Chemical Formula: C6H12O6
Contact Information:
Sciencelab.com, Inc.
14225 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients
Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dextrose anhydrous</td>
<td>50-99-7</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Not applicable.

Section 3: Hazards Identification
Potential Acute Health Effects: Slightly hazardous in case of eye contact (irritant), of ingestion, of inhalation.
Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures
Eye Contact: Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used.
Skin Contact: No known effect on skin contact, rinse with water for a few minutes.
Serious Skin Contact: Not available.
Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.
Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.
Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.
Auto-Ignition Temperature: Not available.
Flash Points: Not available.
Flammable Limits: Not available.
Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards In Presence of Various Substances: Not available.
Explosion Hazards In Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evaporate through the sanitary system. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. If ingested, seek medical advice immediately and show the container or the label.

Storage:
Keep container dry. Keep in a cool place. Ground all equipment containing material. Keep container tightly closed. Keep in a cool, well-ventilated place. Combustible materials should be stored away from extreme heat and away from strong oxidizing agents.

Section 8: Exposure Controls/Personal Protection
Section XII: Appendices

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection: Safety glasses. Lab coat.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 300 (ppm) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.
Odor: Not available.
Taste: Not available.
Molecular Weight: 180.16 g/mole
Color: Not available.
pH (1% soln/water): Not available.
Boiling Point: Decomposes.
Melting Point: 146°C (294.8°F)
Critical Temperature: Not available.
Specific Gravity: 1.562 (Water = 1)
Vapor Pressure: Not applicable.
Vapor Density: Not available.
Volutility: Not available.
Odor Threshold: Not available.
Water/Oil Dist. Coeff.: Not available.
Ionicity (in Water): Not available.
Dispersion Properties: See solubility in water.
Solubility: Easily soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances: Not available.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Not available.
**Section 11: Toxicological Information**

- Routes of Entry: Not available.
- Toxicity to Animals: Acute oral toxicity (LD50): 25,500 mg/kg [Rat].
- Chronic Effects on Humans: Not available.
- Other Toxic Effects on Animals: Slightly hazardous in case of ingestion, of inhalation.
- Special Remarks on Toxicity to Animals: Not available.
- Special Remarks on Chronic Effects on Humans: Passes through the placental barrier in human.
- Special Remarks on other Toxic Effects on Humans: Not available.

**Section 12: Ecological Information**

- Ecotoxicity: Not available.
- BOD5 and COD: Not available.
- Products of Biodegradation: Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
- Toxicity of the Products of Biodegradation: The products of degradation are more toxic.
- Special Remarks on the Products of Biodegradation: Not available.

**Section 13: Disposal Considerations**

- Waste Disposal:

**Section 14: Transport Information**

- DOT Classification: Not a DOT controlled material (United States).
- Identification: Not applicable.
- Special Provisions for Transport: Not applicable.

**Section 15: Other Regulatory Information**

- Federal and State Regulations: TSCA 8(b) Inventory: Dextrose anhydrous
- Other Regulations: Not available.
- Other Classifications:
  - WHMIS (Canada): Not controlled under WHMIS (Canada).
  - DSCL (EEC):
    - This product is not classified according to the EU regulations.
- HMIS (U.S.A.):
Health Hazard: 1
Fire Hazard: 1
Reactivity: 0
Personal Protection: a
National Fire Protection Association (U.S.A.):  
Health: 1
Flammability: 1
Reactivity: 0
Specific hazard:  
Protective Equipment:  
Not applicable. Lab coat. Not applicable. Safety glasses.

Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/11/2005 11:46 AM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Sorbitol MSDS

Section 1: Chemical Product and Company Identification

Product Name: Sorbitol
Catalog Codes: SLS1441, SLS2860
CAS#: 50-70-4
RTECS: LZ4290000
TSCA: TSCA 8(b) Inventory: Sorbitol
Cl#: Not available.
Synonym: D-Glucono
Chemical Name: Not available.
Chemical Formula: C6H14O6

Contact Information:
Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sorbitol</td>
<td>50-70-4</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Sorbitol: ORAL (LD50): Acute: 15900 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
Section XII: Appendices

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.
Auto-Ignition Temperature: Not available.
Flash Points: Not available.
Flammable Limits: Not available.
Products of Combustion: These products are carbon oxides (CO, CO2).
Fire Hazards In Presence of Various Substances: Not available.

Explosion Hazards In Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.
Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evaporate through the sanitary system.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Avoid contact with eyes. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label.

Storage:
Keep container dry. Keep in a cool place. Ground all equipment containing material. Keep container tightly closed. Keep in a cool, well-ventilated place. Combustible materials should be stored away from extreme heat and away from strong oxidizing agents.
Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.
Odor: Not available.
Taste: Not available.
Molecular Weight: 182.17 g/mole
Color: Not available.

pH (1% soln/water): Not available.
Boiling Point: Decomposes.
Melting Point: 111.5°C (232.7°F)
Critical Temperature: Not available.
Specific Gravity: 1.489 (Water = 1)
Vapor Pressure: Not applicable.
Vapor Density: Not available.
Volatile: Not available.
Odor Threshold: Not available.
Water/Oil Dist. Coeff.: Not available.
Ionicty (in Water): Not available.
Dispersion Properties: See solubility in water.
Solubility: Easily soluble in cold water, not water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances: Not available.
Corrosivity: Non-corrosive in presence of glass.
Section XII: Appendices

Section 11: Toxicological Information

Routes of Entry: Eye contact. Ingestion.
Toxicity to Animals: Acute oral toxicity (LD50): 15900 mg/kg [Rat].
Chronic Effects on Humans: Not available.
Other Toxic Effects on Humans: Hazardous in case of ingestion. Slightly hazardous in case of skin contact (Irritant), of Inhalation.
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans: Not available.
Special Remarks on Other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.
BOD5 and COD: Not available.
Products of Biodegradation: Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The products of degradation are more toxic.
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Not a DOT controlled material (United States).
Identification: Not applicable.
Special Provisions for Transport: Not applicable.

Section 15: Other Regulatory Information

Federal and State Regulations: TSCA 8(b) Inventory: Sorbitol
Other Regulations: Not available...
Other Classifications:
WHMIS (Canada): Not controlled under WHMIS (Canada).
DSCL (EEC): R36- Irritating to eyes.
HMIS (U.S.A.):
  Health Hazard: 2
  Fire Hazard: 1
  Reactivity: 0
  Personal Protection: E

National Fire Protection Association (U.S.A.):
  Health: 2
  Flammability: 1
  Reactivity: 0
  Specific hazard:

Protective Equipment:
  Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Splash goggles.

Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/09/2005 06:37 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
p-Xylene MSDS

Section 1: Chemical Product and Company Identification

Product Name: p-Xylene
Catalog Codes: SLX1120
CAS#: 106-42-3
RTECS: ZE2825000
TSCA: TSCA (b) inventory: p-Xylene
CIF: Not applicable.
Synonym: p-Methyltoluene
Chemical Name: 1,4-Dimethylbenzene
Chemical Formula: C₆H₄(CH₃)₂

Contact Information:
Scientelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77393
US Sales: 1-800-991-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Composition</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>(p-)Xylene</td>
<td>106-42-3</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: p-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.]. DERMAL (LD50): Acute: 12400 mg/kg [Rabbit.]. VAPOR (LC50): Acute: 4550 ppm 4 hour(s) [Rat.]

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Irritation of the eye is characterized by redness, watering, and itching. Skin irritation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures
Eye Contact: Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an ointment. If irritation persists, seek medical attention. Wash contaminated clothing before reuse.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation: Not available.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.
Auto-Ignition Temperature: 527°C (980.6°F)
Flash Points: CLOSED CUP: 25°C (77°F), OPEN CUP: 28.9°C (84°F) (Cleveland).
Flammable Limits: LOWER: 1.1% UPPER: 7%
Products of Combustion: These products are carbon oxides (CO, CO2).
Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards:
Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Toxic flammable liquid, insoluble or very slightly soluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas, dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage
Section XII: Appendices

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/vapour/spray. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash gogges. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash gogges. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIH Consult local authorities for acceptable exposure levels.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)
Odor: Not available.
Taste: Not available.
Molecular Weight: 106.17 g/mole
Color: Colorless.
pH (1% soln/water): Not applicable.
Boiling Point: 138°C (280.4°F)
Melting Point: 12°C (53.6°F)
Critical Temperature: Not available.
Specific Gravity: 0.86 (Water = 1)
Vapor Pressure: 9 mm of Hg (@ 20°C)
Vapor Density: 3.7 (Air = 1)
Volatile: Not available.
Odor Threshold: 0.62 ppm
Water/Oil Dist. Coeff.: Not available.
Ionicity (in Water): Not available.
Dispersion Properties: See solubility in water, methanol, diethyl ether.
### Section 10: Stability and Reactivity Data

**Stability:** The product is stable.
**Instability Temperature:** Not available.
**Conditions of Instability:** Not available.
**Incompatibility with various substances:** Reactive with oxidizing agents.
**Corrosivity:** Non-corrosive in presence of glass
**Special Remarks on Reactivity:** Not available.
**Special Remarks on Corrosivity:** Not available.
**Polymerization:** No.

### Section 11: Toxicological Information

**Routes of Entry:** Eye contact.
**Toxicity to Animals:**
*WARNING*: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 5000 mg/kg [Rat]. Acute dermal toxicity (LD50): 12400 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 4650 ppm 4 hour(s) [Rat].

**Chronic Effects on Humans:** The substance is toxic to blood, kidneys, the nervous system, liver.
**Other Toxic Effects on Humans:**
Very hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation.
**Special Remarks on Toxicity to Animals:** Not available.
**Special Remarks on Chronic Effects on Humans:**
0347 Animal: embryo toxic, foetotoxic, passes through the placental barrier. 0690 Detected in maternal milk in human. Narcotic effect: may cause nervous system disturbances.
**Special Remarks on Other Toxic Effects on Humans:** Material is irritating to mucous membranes and upper respiratory tract.

### Section 12: Ecological Information

**Ecotoxicity:** Not available.
**BOD5 and COD:** Not available.
**Products of Biodegradation:**
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
**Toxicity of the Products of Biodegradation:** The products of degradation are more toxic.
**Special Remarks on the Products of Biodegradation:** Not available.

### Section 13: Disposal Considerations

p. 4
Section XII: Appendices

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid.
Identification: Xylene: UN1307 PG: III
Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK; p-Xylene Florida; p-Xylene Massachusetts RTK; p-Xylene New Jersey; p-Xylene TSCA 8(b) inventory; p-Xylene SARA 313 toxic chemical notification and release reporting; p-Xylene CERCLA: Hazardous substances.; p-Xylene


Other Classifications:
WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2B: Material causing other toxic effects (TOXIC).


HMIS (U.S.A.):
Health Hazard: 2
Fire Hazard: 3
Reactivity: 0
Personal Protection: h

National Fire Protection Association (U.S.A.):
Health: 2
Flammability: 3
Reactivity: 0
Specific hazard:

Protective Equipment:
Gloves: Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:
Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
m-Xylene MSDS

Section 1: Chemical Product and Company Identification

| Product Name: m-Xylene          | Contact Information: |
| Catalog Codes: SLX1066          | Sciencelab.com, Inc. |
| CAS#: 108-38-3                  | 14025 Smith Rd.      |
| RTECS: ZE2275000                | Houston, Texas 77396 |
| TSCA: TSCA 8(b) inventory: m-Xylene | US Sales: 1-800-901-7247 |
| Cfl: Not applicable.             | International Sales: 1-281-441-4400 |
| Synonym: m-Methyltoluene        | Order Online: ScienceLab.com |
| Chemical Name: 1,3-Dimethylbenzene | CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300 |
| Chemical Formula: C6H4(CH3)2     | International CHEMTREC, call: 1-703-527-3887 |

Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m-)Xylene</td>
<td>108-38-3</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: m-Xylene: ORAL (LD50): Acute: 5000 mg/kg [Rat.], DERMAL (LD50): Acute: 14100 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant). Slightly hazardous in case of skin contact (permeator), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to blood, kidneys, the nervous system, liver. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

p. 1
Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 527°C (980°F)

Flash Points: CLOSED CUP: 25°C (77°F), OPEN CUP: 28.9°C (84°F) (Cleveland).

Flammable Limits: LOWER: 1.1% UPPER: 7%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Highly flammable in presence of open flames and sparks, of heat.


Fire Fighting Media and Instructions: Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Explosive in the form of vapor when exposed to heat or flame. Vapor may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits acrid smoke and irritating fumes.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill: Flammable liquid, insoluble in water. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not get water inside container. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage
Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/lumes/vapour/spray. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibilities such as oxidizing agents.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls / Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) TWA: 434 STEL: 651 (mg/m3) from ACGIH Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid. (Liquid.)
Odor: Not available.
Taste: Not available.
Molecular Weight: 106.17 g/mole
Color: Colorless.

pH (1% soln/water): Not applicable.
Boiling Point: 139.3°C (282.7°F)
Melting Point: -47.8°F (-54.2°C)

Critical Temperature: Not available.
Specific Gravity: 0.86 (Water = 1)
Vapor Pressure: 8 mm of Hg (@ 20°C)
Vapor Density: 3.7 (Air = 1)
Volatility: Not available.
Odor Threshold: 0.62 ppm
Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.
Dispersion Properties: See solubility in water, methanol, diethyl ether.

Solubility:
Easily soluble in methanol, diethyl ether. Insoluble in cold water, hot water.
Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances: Reactive with oxidizing agents.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Not available.
Special Remarks on Corrosivity: Not available.
Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact.
Toxicity to Animals:
Acute oral toxicity (LD50): 5000 mg/kg [Rat]. Acute dermal toxicity (LD50): 14100 mg/kg [Rabbit].
Chronic Effects on Humans: The substance is toxic to blood, kidneys, the nervous system, liver.
Other Toxic Effects on Humans:
Very hazardous in case of skin contact (irritant). Slightly hazardous in case of skin contact (permeator). of ingestion. of irritation.
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans:
0347 Animal: embryotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect; may cause nervous system disturbances.
Special Remarks on other Toxic Effects on Humans: Material is irritating to mucous membranes and upper respiratory tract.

Section 12: Ecological Information

Ecotoxicity: Not available.
BOD5 and COD: Not available.
Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The products of degradation are more toxic.
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: Class 3: Flammable liquid
Identification: Xylene: UN1307 PG: III
Section XII: Appendices

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: m-Xylene Massachusetts RTK: m-Xylene TSCA 8(b) inventory: m-Xylene SARA 313 toxic chemical notification and release reporting: m-Xylene CERCLA: Hazardous substances: m-Xylene


Other Classifications:
WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EFC): R10- Flammable. R38- Irritating to skin. R41- Risk of serious damage to eyes.

HMS (U.S.A.):
Health Hazard: 2
Fire Hazard: 3
Reactivity: 0
Personal protection:

National Fire Protection Association (U.S.A.):
Health: 2
Flammability: 3
Reactivity: 0
Specific hazard:

Protective Equipment:
Gloves. Lab coat. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:

Other Special Considerations: Not available.

Created: 10/10/2005 08:33 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
o-Xylene MSDS

Section 1: Chemical Product and Company Identification

<table>
<thead>
<tr>
<th>Product Name:</th>
<th>o-Xylene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalog Codes:</td>
<td>SLX1012</td>
</tr>
<tr>
<td>CAS#:</td>
<td>95-47-6</td>
</tr>
<tr>
<td>RTECS:</td>
<td>ZE2450000</td>
</tr>
<tr>
<td>TSCA:</td>
<td>TSCA (b) Inventory: o-Xylene</td>
</tr>
<tr>
<td>C#</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Synonym</td>
<td>1,2-Dimethylbenzene</td>
</tr>
<tr>
<td>Chemical Name:</td>
<td>o-Xylene</td>
</tr>
<tr>
<td>Chemical Formula:</td>
<td>C6H4(CH3)2</td>
</tr>
</tbody>
</table>

Contact Information:
Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77366
US Sales: 1-806-961-7247
International Sales: 1-281-441-4400
Order Online: Scienclab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-5300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>(o-)Xylene</td>
<td>95-47-6</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: o-Xylene LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

Potential Acute Health Effects: Hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal) by ACGIH, 3 (Not classifiable for human) by IARC.
MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/male [POSSIBLE]. The substance may be toxic to kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Section XII: Appendices

Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Get medical attention.

**Skin Contact:**
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

**Serious Skin Contact:**
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

**Inhalation:**
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

**Serious Inhalation:**
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

**Ingestion:**
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

**Serious Ingestion:** Not available.

---

**Section 5: Fire and Explosion Data**

**Flammability of the Product:** Flammable.
**Auto-Ignition Temperature:** 453°C (865.4°F)
**Flash Points:** CLOSED CUP: 17°C (62.6°F)
**Flammable Limits:** LOWER: 0.9% UPPER: 6.7%
**Products of Combustion:** These products are carbon oxides (CO, CO₂).

**Fire Hazards in Presence of Various Substances:** Highly flammable in presence of open flames and sparks, of heat.

**Explosion Hazards in Presence of Various Substances:**
Risks of explosion of the product in presence of mechanical impact: Not available. Slightly explosive in presence of open flames and sparks, of heat.

**Fire Fighting Media and Instructions:**
Flammable liquid, insoluble in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog.

**Special Remarks on Fire Hazards:**
Vapors are heavier than air and may travel considerable distance to source of ignition and flash back. When heated to decomposition it emits toxic smoke and irritating fumes.

**Special Remarks on Explosion Hazards:**
Explosive in the form of vapor when exposed to heat or flame. Vapors may form explosive mixtures with air. Containers may explode when heated. Runoff to sewer may create fire or explosion hazard.

---

**Section 6: Accidental Release Measures**

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**

---

299
### Section 7: Handling and Storage

**Precautions:**
Keep locked up. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/steam/vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

**Storage:**
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

### Section 8: Exposure Controls/Personal Protection

**Engineering Controls:**
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit values. Ensure that eyewash stations and safety showers are proximal to the work-station location.

**Personal Protection:**
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

**Personal Protection in Case of a Large Spill:**
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

**Exposure Limits:**
TWA: 434 STEL: 651 (mg/m3) from ACGIH (TLV) [United States] TWA: 100 STEL: 150 (ppm) from ACGIH (TLV) [United States] STEL: 150 (ppm) from NIOSH STEL: 655 (mg/m3) from NIOSH Consult local authorities for acceptable exposure limits.

### Section 9: Physical and Chemical Properties

**Physical state and appearance:** Liquid. (Mobile, nonpolar liquid.)
**Odor:** Aromatic. Sweetish.
**Taste:** Not available.
**Molecular Weight:** 106.17 g/mole
**Color:** Colorless.
**pH (1% soln/water):** Not applicable.
**Boiling Point:** 144.4°C (291.9°F)
**Melting Point:** -25°C (-13°F)
**Critical Temperature:** 359°C (678.2°F)
**Specific Gravity:** 0.68 (Water = 1)
**Vapor Pressure:** 0.9 kPa (@ 20°C)
**Vapor Density:** 3.7 (Air = 1)
Section XII: Appendices

Volutiy: Not available.
Odor Threshold: 0.05 ppm
Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 3.1
Ionicity (in Water): Not available.
Dispersion Properties:
Dispensed in diethyl ether. Is not dispersed in cold water, hot water. See solubility in diethyl ether, acetone.
Solubility:
Soluble in diethyl ether, acetone. Insoluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Incompatibility with various substances: Reactive with oxidizing agents, acids.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity:
Photochemically reactive. Incompatible with strong oxidizers (e.g., chlorine, bromine, fluorine), and strong acids (e.g., nitric acid, acetic acid).
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact: Eye contact. Inhalation.
Toxicity to Animals:
Lowest Published Lethal Dose - Inhalation (LCL): 6125 ppm 12 hours [Rat]; 6125 ppm 12 hours [Human] Lowest Published Lethal Dose - Oral: 5000 mg/kg [Rat]
Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC.
TERATOGENIC EFFECTS: Classified POSSIBLE for human. DEVELOPMENTAL TOXICITY: Classified Reproductive system/ toxinnmale [POSSIBLE] May cause damage to the following organs: kidneys, liver, upper respiratory tract, skin, eyes, central nervous system (CNS).
Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant, permeator). of ingestion, of inhalation.
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (male) and birth defects based on animal data. 0247 Animal: embritotoxic, foetotoxic, passes through the placental barrier. 0900 Detected in maternal milk in human. Narcotic effect, may cause nervous system disturbances.
Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects Skin: May cause skin irritation. May be absorbed through skin in harmful amounts. Eyes: Causes severe eye irritation. Inhalation: Causes respiratory tract and mucous membranes irritation. May affect sense organs, behavior (Central Nervous system) which may result in dizziness, general weakness, central nervous system depression, confusion, ataxia, disorientation, lethargy, drowsiness, headaches. May also affect respiration, cardiovascular system, liver, blood, and digestive system (nausea, vomiting) ingestion: Harmful if swallowed. Causes digestive tract irritation with nausea, vomiting
and diarrhea. May also affect metabolism, liver, and urinary system, and central nervous system (excitement followed by headache, dizziness, drowsiness and nausea). Chronic Potential Health Effects: Skin: Prolonged or repeated contact may cause dermatitis or permanent eye damage. Inhalation: Chronic inhalation may cause effects similar to those of acute inhalation.

### Section 12: Ecological Information

Ecotoxicity: Not available.

**BOD5 and COD:** Not available.

**Products of Biodegradation:**
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

**Toxicity of the Products of Biodegradation:** The products of degradation are less toxic than the product itself.

**Special Remarks on the Products of Biodegradation:** Not available.

### Section 13: Disposal Considerations

**Waste Disposal:**
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

### Section 14: Transport Information

**DOT Classification:** CLASS 3: Flammable liquid.

**Identification:** : Xylene UNNA: 1307 PG: II

**Special Provisions for Transport:** Not available.

### Section 15: Other Regulatory Information

**Federal and State Regulations:**

**Other Regulations:**

**Other Classifications:**
WHMIS (Canada): CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

**DSL (EEC):**

**HMIS (U.S.A.):**
- Health Hazard: 2
- Fire Hazard: 3
Section XII: Appendices

Reactivity: 0
Personal Protection: h
National Fire Protection Association (U.S.A.):
  Health: 2
  Flammability: 3
  Reactivity: 0
  Specific hazard:
Protective Equipment:
  Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References:

Other Special Considerations: Not available.
Created: 10/11/2005 12:54 PM
Last Updated: 1/1/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Benzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Benzene
Catalog Codes: SLB1564, SLB3055, SLB2881
CAS#: 71-43-2
RTECS: CY1400000
TSCA: TSCA 8(b) Inventory: Benzene
Cl#: Not available.
Synonym: Benzol; Benzene
Chemical Name: Benzene
Chemical Formula: C6H6
Contact Information:
Scioncolab.com, Inc.
14025 Smith Rd.
Houston, Texas 77356
US Sales: 1-800-961-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>71-43-2</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Benzene: ORAL (LD50): Acute: 930 mg/kg [Rat], 4700 mg/kg [Mouse]. DERMAL (LD50): Acute: 8400 mg/kg [Rabbit]. VAPOR (LC50): Acute: 10000 ppm 7 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. The substance is toxic to blood, bone marrow, central nervous system (CNS). The substance may be toxic to liver, Urinary System. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures
Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention if symptoms appear.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

---

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.
Auto-Ignition Temperature: 497.78°C (928°F)
Flash Points: CLOSED CUP: -11.1°C (12°F). (SetoFlash)
Flammable Limits: LOWER: 1.2% UPPER: 7.8%
Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances:
Highly flammable in presence of open flames and sparks, of heat. Slightly flammable to flammable in presence of oxidizing materials. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards:
Extremely flammable liquid and vapor. Vapor may cause flash fire. Reacts on contact with iodine heptafluoride gas. Dioxygenyl tetrifuoroborate is as very powerful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition. Contact with sodium peroxyd with benzene causes ignition. Benzene ignites in contact with powdered chrome anhydride. Vigorous or inconspicuous reaction with hydrogen + Raney nickel (above 210°C) and bromine trifluoride.

Special Remarks on Explosion Hazards:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitrile perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction
of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimanganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powerful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxodisulfuric acid with benzene explodes.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas, dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States] TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States] TWA: 0.1 STEL: 1 from NIOSH TWA: 1 STEL: 5 (ppm) from OSHA (PEL) [United States] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 3 (ppm) [United Kingdom (UK)] TWA: 1.6 (mg/m3) [United Kingdom (UK)] TWA: 1 (ppm) [Canada] TWA: 3.2 (mg/m3) [Canada] TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor:
Aromatic. Gasoline-like, rather pleasant. (Strong)

Taste:
Not available.

Molecular Weight: 78.11 g/mole
Section XII: Appendices

Color: Clear Colorless. Colorless to light yellow.
P.H (1% soln/water): Not available.
Boiling Point: 80.1 (176.2°F)
Melting Point: 5.5°C (41.9°F)
Critical Temperature: 286.9°C (552°F)
Specific Gravity: 0.8787 @ 15 C (Water = 1)
Vapor Pressure: 10 kPa (@ 20°C)
Vapor Density: 0.28 (Air = 1)
Volatile: Not available.
Odor Threshold: 4.68 ppm
Water/Oil Dist. Coeff.: The product is more soluble in oil, log(oil/water) = 2.1
Ioncity (in Water): Not available.
Dispersion Properties: See solubility in water, diethyl ether, acetone.
Solubility: Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Heat, ignition sources, incompatibles.
Incompatibility with various substances: Highly reactive with oxidizing agents, acids.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentfluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentfluoride and methoxide (from arsenic pentfluoride and potassium methoxide) in trichlorofluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimanganic heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powerful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxythiosulfuric acid with benzene explode.
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 930 mg/kg [Rat]. Acute dermal toxicity (LD50): >9430 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 16600 7 hours [Rat].

Chronic Effects on Humans:

DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. Causes damage to the following organs: blood, bone marrow, central nervous system (CNS). May cause damage to the following organs: liver, Urinary System.

Other Toxic Effects on Humans:
Very hazardous in case of inhalation. Hazardous in case of skin contact (iritant, permeator), of ingestion.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic, leukemia). Human: passes the placental barrier, detected in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism, and urinary system. Eyes: Causes eye irritation. Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/Central and Peripheral nervous systems (somnia, muscle weakness, general anesthetic, and other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system. Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood.

Section 12: Ecological Information

Ecotoxicity: Not available.
BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3. Flammable liquid.
Identification: Benzene UNNA: 1114 PG: II
Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene California prop. 65 (no significant risk level). Benzene: 0.007 mg/day (value) California prop. 65: This product contains the following ingredients
for which the State of California has found to cause cancer which would require a warning under the statute: Benzene Connecticut carcinogen reporting list: Benzene Connecticut hazardous material survey: Benzene Illinois toxic substances disclosure to employee act: Benzene New York release reporting list: Benzene Rhode Island RTK hazardous substances: Benzene Pennsylvania RTK: Benzene Minnesota: Benzene Michigan critical material: Benzene Massachusetts RTK: Benzene Massachusetts spill list: Benzene New Jersey: Benzene New Jersey spill list: Benzene Louisiana spill reporting: Benzene California Director's list of Hazardous Substances: Benzene TSCA 8(b) Inventory: Benzene SARA 313 toxic chemical notification and release reporting: Benzene CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.556 kg)

Other Regulations:

Other Classifications:
WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):

HMIS (U.S.A.):
Health Hazard: 2
Fire Hazard: 3
Reactivity: 0
Personal Protection: h

National Fire Protection Association (U.S.A.):
Health: 2
Flammability: 3
Reactivity: 0
Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/10/2005 08:35 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Toluene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Toluene
Catalog Codes: SLT2857, SLT3277
CAS#: 108-88-3
RTECS: X55250000
TSCA: TSCA 8(b) inventory; Toluene
GHS: Not available.
Synonym: Toluol, Tolu-Sol; Methylbenzene; Methadex; Phenylmethane, Methylbenzol
Chemical Name: Toluene
Chemical Formula: C8-H8-CH3 or C7-H8

Contact Information:
 ScienceLab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-881-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS#</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Toluene: ORAL (LD50): Acute: 636 mg/kg [Rat]. DERMAL (LD50): Acute: 14100 mg/kg [Rabbit]. VAPOR (LC50): Acute: 45000 ppm 4 hours [Rat]. 440 ppm 24 hours [Mouse].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permuter).

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC
MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, kidneys, the nervous system, liver, brain, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures
Section XII: Appendices

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.
Auto-Ignition Temperature: 460°C (860°F)
Flash Points: CLOSED CUP: 4.444°C (40°F), (Setatlash) OPEN CUP: 16°C (60.9°F).
Flammable Limits: LOWER: 1.1% UPPER: 7.1%
Products of Combustion: These products are carbon oxides (CO, CO2)

Fire Hazards in Presence of Various Substances:
Flammable in presence of open flames and sparks, of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, insoluble in water: SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards:
Toluene forms explosive reaction with 1,3-dichloro-5,5-dimethyl-2,4-imidazolidione; dinitrogen tetraoxide; concentrated nitric acid, sulfuric acid + nitric acid. N2O4, AgClO4, BrF3; Uranium hexafluoride; sulfur dichloride. Also forms an explosive mixture with tetranitromethane.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

p. 2
Section 7: Handling and Storage

Procedures:
- Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/cloud/vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents.

Storage:
- Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
- Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
- Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
- Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient, consult a specialist BEFORE handling this product.

Exposure Limits:
- TWA: 200 STEL: 500 CEIL: 300 (ppm) from OSHA (PEL) [United States] TWA: 50 (ppm) from ACGIH (TLV) [United States] SKIN TWA: 100 STEL: 150 (mg/m3) from NIOSH [United States] TWA: 375 STEL: 560 (mg/m3) from NIOSH [United States] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.
Odor: Sweet, pungent, Benzene-like.
Taste: Not available.
Molecular Weight: 92.14 g/mole
Color: Colorless.
pH (1% soln/water): Not applicable.
Boiling Point: 110.6°C (231.1°F)
Melting Point: -95°C (-139°F)
Critical Temperature: 318.6°C (605.5°F)
Specific Gravity: 0.8638 (Water = 1)
Section XII: Appendices

Vapor Pressure: 3.8 kPa (@ 25°C)
Vapor Density: 3.1 (Air = 1)
Volatility: Not available.
Odor Threshold: 1.6 ppm
Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 2.7
Toricity (in Water): Not available.
Dispersion Properties: See solubility in water, diethyl ether, acetone.
Solubility:
- Soluble in diethyl ether, acetone. Practically insoluble in cold water. Soluble in ethanol, benzene, chloroform, glacial acetic acid, carbon disulfide. Solubility in water: 0.561 g/l @ 25 deg. C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Heat, ignition sources (flames, sparks, static), incompatible materials
Incompatibility with various substances: Reactive with oxidizing agents.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity:
- Incompatible with strong oxidizers, silver perchlorate, sodium difluoride, Tetranitromethane, Uranium Hexafluoride. Frozen Bromine Trifluoride reacts violently with Toluene at -80 deg. C. Reacts chemically with nitrogen oxides, or halogens to form nitrotoluene, nitrobenezene, and nitrophenol and halogenated products, respectively.
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.
Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 630 mg/kg [Rat]. Acute dermal toxicity (LD50): 14100 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 440 24 hours [Mouse].
Chronic Effects on Humans:
Carcinogenic Effects: A4 (Not classifiable for human or animal.) by ACGIH, 3 (Not classifiable for human.) by IARC. May cause damage to the following organs: blood, kidneys, the nervous system, liver, brain, central nervous system (CNS).
Other Toxic Effects on Humans:
- Hazardous in case of skin contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).
Special Remarks on Toxicity to Animals:
- Lowest Published Lethal Dose: LD50 [Human] - Route: Oral, Dose: 50 mg/kg LCL [Rabbit] - Route: Inhalation, Dose: 55000 ppm/40min
Special Remarks on Chronic Effects on Humans:
- Detected in maternal milk in human. Passes through the placental barrier in human. Embryotoxic and/or foetotoxic in animal. May cause adverse reproductive effects and birth defects (teratogenic). May affect genetic material (mutagenic).
Special Remarks on Other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes mild to moderate skin irritation. It can be absorbed to some extent through the skin. Eyes: Causes mild to moderate eye irritation with a burning sensation. Splash contact with eyes also causes conjunctivitis, blepharospasm, corneal edema, corneal abrasions. This usually resolves in 2 days. Inhalation: Inhalation of vapor may cause respiratory tract irritation causing coughing and wheezing, and nasal discharge. Inhalation of high concentrations may affect behavior and cause central nervous system effects characterized by nausea, headache, dizziness, tremors, restlessness, lightheadedness, exhilaration, memory loss, insomnia, impaired reaction time, drowsiness, ataxia, hallucinations, somnolence, muscle contraction or spasticity, unconsciousness and coma. Inhalation of high concentration of vapor may also affect the cardiovascular system (rapid heart beat, heart palpitations, increased or decreased blood pressure, dysrhythmia). Respiration (acute pulmonary edema, respiratory depression, apnea, asphyxia). Cause vision disturbances and dilated pupils, and cause loss of appetite. Ingestion: Aspiration hazard. Aspiration of Toluene into the lungs may cause chemical pneumonitis. May cause irritation of the digestive tract with nausea, vomiting, pain. May have effects similar to that of acute inhalation. Chronic Potential Health Effects: Inhalation and Ingestion: Prolonged or repeated exposure via inhalation may cause central nervous system and cardiovascular symptoms similar to that of acute inhalation and ingestion as well liver damage/failure, kidney damage/failure (with hematuria, proteinuria, oliguria, renal tubular acidosis), brain damage, weight loss, blood (pigmented or nucleated red blood cells, changes in white blood cell count), bone marrow changes, electrolyte imbalances (Hypokalemia, Hypophosphatemia), severe, muscle weakness and Rhabdomyolysis. Skin: Repeated or prolonged skin contact may cause defatting dermatitis.

### Section 12: Ecological Information

**Ecotoxicity:**
Ecotoxicity in water (LC50): 313 mg/l 48 hours [Laphnia (daphnia)], 17 mg/l 24 hours [Fish (Blue Gill)], 13 mg/l 96 hours [Fish (Blue Gill)]. 55 mg/l 24 hours [Fish (Fathead minnow)], 34 mg/l 96 hours [Fish (Fathead minnow)], 56.8 ppm any hours [Fish (Goldfish)].

**BODS and COD:** Not available.

**Products of Biodegradation:**
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

**Toxicity of the Products of Biodegradation:** The products of degradation are less toxic than the product itself.

**Special Remarks on the Products of Biodegradation:** Not available.

### Section 13: Disposal Considerations

**Waste Disposal:**
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

### Section 14: Transport Information

**DOT Classification:** CLASS 3: Flammable liquid.

**Identification:** Toluene UNNA: 1294 PG: II

**Special Provisions for Transport:** Not available.

### Section 15: Other Regulatory Information

**Federal and State Regulations:**
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Toluene California prop. 65 (no significant risk level): Toluene: 7 mg/day (value) California prop. 65 (acceptable daily intake level): Toluene: 7 mg/day (value)

California prop. 65: This product contains the following ingredients for which the State of California has found to cause birth defects which would require a warning under the statute: Toluene Connecticut hazardous material survey: Toluene Illinois...
Section XII: Appendices

Section 16: Other information

References: Not available.
Other Special Considerations: Not available.
Created: 10/10/2005 08:30 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Naphthalene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Naphthalene
Catalog Codes: SLN1789, SLN2401
CAS#: 91-20-3
RTECS: QJ0525000
TSCA: TSCA 8(b) Inventory: Naphthalene
CIF: Not available.
Synonym:
Chemical Name: Not available.
Chemical Formula: C10H8

Contact Information:
Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77395
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: Sciencelab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3867
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naphthalene</td>
<td>91-20-3</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Naphthalene:
- ORAL (LD50): Acute: 490 mg/kg [Rat], 533 mg/kg [Mouse], 1200 mg/kg [Guinea pig],
- DERMAL (LD50): Acute: 20001 mg/kg [Rabbit],
- VAPOR (LC50): Acute: 170 ppm 4 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of ingestion, Hazardous in case of eye contact (irritant), of inhalation. Slightly hazardous in case of skin contact (irritant, permeator). Severe over-exposure can result in death.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal) by ACGIH. MUTAGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Development toxic (POSSIBLE). The substance is toxic to blood, kidneys, the nervous system, the reproductive system, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures
Section XII: Appendices

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact: Not available.

Inhalation: Allow the victim to rest in a well ventilated area. Seek medical attention immediately.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen light clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.
Auto-Ignition Temperature: 567°C (1052.6°F)
Flammable Limits: LOWER: 0.9% UPPER: 5.9%
Products of Combustion: These products are carbon oxides (CO, CO2).
Fire Hazards in Presence of Various Substances: Not available.
Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.
Fire Fighting Media and Instructions:
Flammable solid. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.
Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Flammable solid. Stop leak if without risk. Do not touch spilled material. Use water spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.
### Section 7: Handling and Storage

**Precautions:**
Keep locked up. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe dust. Avoid contact with eyes. Wear suitable protective clothing in case of insufficient ventilation, wear suitable respiratory equipment if ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibilities such as oxidizing agents.

**Storage:**
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

### Section 8: Exposure Controls/Personal Protection

**Engineering Controls:**
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

**Personal Protection:**
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

**Personal Protection in Case of a Large Spill:**
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

**Exposure Limits:**

### Section 9: Physical and Chemical Properties

**Physical state and appearance:** Solid. (Crystalline solid.)

**Odor:** Aromatic.

**Taste:** Not available.

**Molecular Weight:** 128.19 g/mole

**Color:** White.

**pH (1% soln/water):** Not available.

**Boiling Point:** 218°C (424.4°F)

**Melting Point:** 80.2°C (176.4°F)

**Critical Temperature:** Not available.

**Specific Gravity:** 1.162 (Water = 1)

**Vapor Pressure:** Not applicable.

**Vapor Density:** 4.4 (Air = 1)

**Volatility:** Not available.

**Odor Threshold:** 0.038 ppm

**Water/Oil Dist. Coeff.:** Not available.
Section XII: Appendices

Ionicity (in Water): Not available.
Dispersion Properties:
Partially dispersed in hot water, methanol, n-octanol. Very slightly dispersed in cold water. See solubility in methanol, n-octanol.
Solubility:
Partially soluble in methanol, n-octanol. Very slightly soluble in cold water, hot water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances: Highly reactive with oxidizing agents.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Not available.
Special Remarks on Corrosivity: May attack some forms of rubber and plastic
Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.
Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 490 mg/kg [Rat]. Acute dermal toxicity (LD50): 20001 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 170 ppm 4 hour(s) [Rat].
Chronic Effects on Humans:
CARCINOGENIC EFFECTS: A4 (Not classifiable for human or animal.) by ACGIH. DEVELOPMENTAL TOXICITY: Classified Developmental toxic [POSSIBLE]. The substance is toxic to blood, kidneys, the nervous system, the reproductive system, liver, mucous membranes, gastrointestinal tract, upper respiratory tract, central nervous system (CNS).
Other Toxic Effects on Humans:
Very hazardous in case of ingestion. Hazardous in case of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans: Not available.
Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Ecotoxicity in water (LC50): 305.2 ppm 96 hour(s) [Trout].
BOD5 and COD: Not available.
Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The products of degradation are more toxic.
Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 4.1: Flammable solid.
Identification: Naphthalene, refined: UN1334 PG: III
Special Provisions for Transport: Marine Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
- Rhode Island RTK hazardous substances: Naphthalene Pennsylvania RTK: Naphthalene Florida: Naphthalene Minnesota: Naphthalene Massachusetts RTK: Naphthalene TSCA 9(b) Inventory: Naphthalene TSCA 9(a) PAIR: Naphthalene TSCA 8(d) H and S data reporting: Naphthalene: 06/07 SARA 313 toxic chemical notification and release reporting: Naphthalene: 1%
- CERCLA: Hazardous substances: Naphthalene: 100 lbs. (45.36 kg)

Other Regulations:
- EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:
- WHMIS (Canada):
  - CLASS B-4: Flammable solid. CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC). CLASS D-2B: Material causing other toxic effects (TOXIC).
- DSCCL (EEC):
  - R36- Irritating to eyes. R40- Possible risks of irreversible effects. R48/22- Harmful: danger of serious damage to health by prolonged exposure if swallowed. R49/23- Toxic: danger of serious damage to health by prolonged exposure through inhalation. R63- Possible risk of harm to the unborn child.

HMIS (U.S.A.):
- Health Hazard: 2
- Fire Hazard: 2
- Reactivity: 0
- Personal Protection: E

National Fire Protection Association (U.S.A.):
- Health: 2
- Flammability: 2
- Reactivity: 0
- Specific hazard:

Protective Equipment:
- Gloves: Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.
Section 16: Other Information

References: Not available.
Other Special Considerations: Not available.
Created: 10/11/2005 01:30 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Ethylbenzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Ethylbenzene
Catalog Code: SLE2044
CAS#: 100-41-4
RTECS: DA0700000
TSCA: TSCA (b) inventory: Ethylbenzene
Cl#: Not available.
Synonym: Ethyl Benzene; Ethylbenzol; Phenylethane
Chemical Name: Ethylbenzene
Chemical Formula: C8H10

Contact Information:
Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77395
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: Sciencelab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and information on ingredients

Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylbenzene</td>
<td>100-41-4</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Ethylbenzene: ORAL (LD50): Acute: 3500 mg/kg [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Potential Chronic Health Effects:
Slightly hazardous in case of skin contact (irritant, sensitizer). CARCINOGENIC EFFECTS: Classified 2B (Possible for human.) by IARC. MUTAGENIC EFFECTS: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Section XII: Appendices

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention.

**Skin Contact:** Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops.

**Serious Skin Contact:** Not available.

**Inhalation:**
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

**Serious Inhalation:**
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek medical attention.

**Ingestion:**
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

**Serious Ingestion:** Not available.

### Section 5: Fire and Explosion Data

**Flammability of the Product:** Flammable.

**Auto-Ignition Temperature:** 432°C (800.6°F)

**Flash Points:**
CLOSED CUP: 15°C (59°F), (Tagliabue) OPEN CUP: 36.67°C (90°F) (Cleveland) (CHRIS, 2001) CLOSED CUP: 12.8°C (55°F) (Bingham et al., 2001) NIOSH, 2001) CLOSED CUP: 21°C (70°F) (NFPA)

**Flammable Limits:** LOWER: 0.5% - 1.8% UPPER: 5.7% - 7%

**Products of Combustion:** These products are carbon oxides (CO, CO2).

**Fire Hazards in Presence of Various Substances:** Highly flammable in presence of open flames and sparks, of heat.

**Explosion Hazards in Presence of Various Substances:**

**Fire Fighting Media and Instructions:**
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

**Special Remarks on Fire Hazards:**
Vapor may travel considerable distance to source of ignition and flash back. Vapors may form explosive mixtures with air. When heated to decomposition it emits toxic fumes and irritating fumes.

**Special Remarks on Explosion Hazards:** Vapors may form explosive mixtures in air.

### Section 6: Accidental Release Measures

**Small Spill:** Absorb with an inert material and put the spilled material in an appropriate waste disposal.

**Large Spill:**
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; danger of fire. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.
Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/tumes/vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibilities such as oxidizing agents.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 100 STEL: 125 (ppm) from OSHA (PEL) [United States] TWA: 435 STEL: 545 from OSHA (PEL) [United States] TWA: 435 STEL: 545 (mg/m³) from NIOSH (United States) TWA: 100 STEL: 125 (ppm) from NIOSH (United States) TWA: 100 STEL: 125 (ppm) from ACGIH (TLV) [United States] TWA: 100 STEL: 125 (ppm) [United Kingdom (UK)] TWA: 100 STEL: 125 (ppm) [Belgium] TWA: 100 STEL: 125 (ppm) [Finland] TWA: 50 (ppm) [Norway] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.
Odor: Sweetish, Gasoline-like, Aromatic.
Taste: Not available.
Molecular Weight: 106.16 g/mole
Color: Colorless.
 pH (1% soln/water): Not available.
Boiling Point: 135°C (276.9°F)
Melting Point: -54.9 (-138.8°F)
Critical Temperature: 617.15°C (1142.9°F)
Specific Gravity: 0.667 (Water = 1)
Vapor Pressure: 0.9 kPa (@ 20°C)
Vapor Density: 3.66 (Air = 1)
Vocality: 100% (v/v)
Odor Threshold: 140 ppm
Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/tumes/vapor/spray. Avoid contact with eyes. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibilities such as oxidizing agents.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.
Taste: Not available.
Molecular Weight: 106.16 g/mole
Color: Colorless.
pH (1% soln/water): Not available.
Boiling Point: 135°C (276.9°F)
Melting Point: -54.9 (-130.8°F)
Critical Temperature: 617.15°C (1142.9°F)
Specific Gravity: 0.667 (Water = 1)
Vapor Pressure: 0.9 kPa (@ 20°C)
Vapor Density: 3.66 (Air = 1)
Volatility: 100% (v/v).
Odor Threshold: 140 ppm
Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Heat, ignition sources (flames, sparks, static), incompatible materials, light
Incompatibility with various substances: Reactive with oxidizing agents.
Corrosivity: Not considered to be corrosive for metals and glass.
Special Remarks on Reactivity:
Can react vigorously with oxidizing materials. Sensitive to light.
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin, inhalation.
Toxicity to Animals: Acute oral toxicity (LD50): 3600 mg/kg [Rat].
Chronic Effects on Humans:
Carcinogenic Effects: Classified 2B (Possible for human) by IARC. Mutagenic Effects: Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. May cause damage to the following organs: central nervous system (CNS).
Other Toxic Effects on Humans:
Hazardous in case of ingestion, inhalation. Slightly hazardous in case of skin contact (irritant, permeator).
Special Remarks on Toxicity to Animals:
Lethal Dose/Conc. 50% Kill: LD50 [Rabbit] - Route: Skin, Dose: 17800 u/g Lowest Published Lethal Dose/Conc. LD50 [Rat] - Route: Inhalation (vapor), Dose: 4000 ppm/4 h
Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects and birth defects (teratogenic) based on animal test data. May cause cancer based on animal data. IARC evidence for carcinogenicity in animals is sufficient. IARC evidence of carcinogenicity in humans inadequate. May affect genetic material (mutagenic).
Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Can cause mild skin irritation. It can be absorbed through intact skin. Eyes: Contact with vapor or liquid can cause severe eye irritation depending on concentration. It may also cause conjunctivitis. At a vapor exposure level of 85 - 200 ppm, it is mildly and transiently irritating to the eyes; 1000 ppm causes further irritation and tearing; 2000 ppm results in immediate and severe irritation and tearing; 5,000 ppm is intolerable (ACGIH, 1991; Clayson and Clayson, 1994). Standards established for eye irritation using 500 mg resulted in severe irritation (ITECS) Inhalation: Exposure to high concentrations can cause nasal, mucous membrane and respiratory tract irritation and can also result in chest constriction and trouble breathing, respiratory failure, and even death. It can also affect behavior/Central Nervous System. The effective dose for CNS depression in experimental animals was 10,000 ppm (ACGIH, 1991). Symptoms of CNS depression include
Section XII: Appendices

headache, nausea, weakness, dizziness, vertigo, irritability, fatigue, lightheadedness, sleepiness, tremor, loss of coordination, judgement and consciousness, coma, and death. It can also cause pulmonary edema. Inhalation of 65 ppm can produce fatigue, insomnia, headache, and mild irritation of the respiratory tract (Haley & Bernet, 1987). Ingestion: Do not drink, pipet or siphon by mouth. May cause gastrointestinal/digestive tract irritation with Abdominal pain, nausea, vomiting. Ethylbenzene is a pulmonary aspiration hazard. Pulmonary aspiration of even small amounts of the liquid may cause fatal pneumonitis. It may also affect behavior/central nervous system with

Section 12: Ecological Information

Ecotoxicity:
Ecotoxicity in water (LC50): 14 mg/l 96 hours [Fish (Trout)] (static). 12.1 mg/l 95 hours [Fish (Fathead Minnow)] (flow-through). 150 mg/l 96 hours [Fish (Blue Gill/Sunfish)] (static). 275 mg/l 96 hours [Fish (Sheepshead Minnow)]. 42.3 mg/l 96 hours [Fish (Fathead Minnow)] (soft water). 97.5 mg/l 96 hours [Shrimp].

BOD5 and COD: Not available.

Products of Biodegradation: Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.
Identification: Ethylbenzene UNNA: 1175 PG: II
Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:

Other Regulations:

Other Classifications:
WHIMIS (Canada):
CLA S B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VER Y TOXIC). CLASSE D-2B: Material causing other toxic effects (TOXIC).

p. 5
Section 16: Other Information

References:
- Manufacturer's Material Safety Data Sheet
- Association (NFPA) - Registry of Toxic Effects of Chemical Substances (RTECS) - Chemical Hazard Response Information System (CHRIS) - Hazardous Substance Data Bank (HSDB) - New Jersey Hazardous Substance Fact Sheet - Ariel Global View
- Reprotect System

Other Special Considerations: Not available.

Created: 10/09/2005 05:28 PM
Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Cumene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Cumene
Catalog Codes: SLC3052
CAS#: 108-82-8
RTECS: GR8575000
TSCA: TSCA 8(b) Inventory: Cumene
Confidential: Not Available.
Synonyms: Isopropyl benzene; Cumol; 2-Phenyl propano; (1-Methylethyl)benzene
Chemical Name: Isopropylbenzene
Chemical Formula: C6H5CH(CH3)2

Contact Information:
ScienceLab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-901-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cumene</td>
<td>98-82-8</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Cumene: ORAL (LD50): Acute: 1400 mg/kg [Rat], 12750 mg/kg [Mouse], DERMAL (LD50): Acute: 12300 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (irritant, permeator), of eye contact (irritant), of ingestion, of inhalation. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Very hazardous in case of skin contact (permeator), CARCINOGENIC EFFECTS: Not available, MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, the nervous system, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures
Section 6: Fire and Explosion Data

Flammability of the Product: Flammable.
Auto-Ignition Temperature: 424°C (755.2°F)
Flash Points: CLOSED CUP: 36°C (96.8°F). OPEN CUP: 44°C (111.2°F).
Flammable Limits: LOWER: 0.9% UPPER: 6.5%
Products of Combustion: These products are carbon oxides (CO, CO2)
Fire Hazards in Presence of Various Substances: Flammable in presence of open flames and sparks.
Fire Fighting Media and Instructions: Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.
Special Remarks on Fire Hazards: Not available.
Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill: Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; close if needed. Eliminate all ignition sources. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.
Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not inhale. Do not breathe gas/tumes/vapourspray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. A refrigerated room would be preferable for materials with a flash point lower than 37.8°C (100°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 50 CEIL: 75 (ppm) TWA: 245 CEIL: 385 (mg/m3) Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.
Odor: Not available.
Taste: Not available.
Molecular Weight: 120.2 g/mole
Color: Clear Colorless.
PH (1% soln/water): Not available.
Boiling Point: 152.4°C (306.3°F)
Melting Point: -56°C (-140.8°F)
Critical Temperature: Not available.
Specific Gravity: 0.802 (Water = 1)
Vapor Pressure: 3 mm of Hg (@ 20°C)
Vapor Density: 4.14 (Air = 1)
Volatile: Not available.
Odor Threshold: 1.2 ppm
Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 3.7
Ionicity (In Water): Not available.
Dispersion Properties: Not available.
Solubility: Very slightly soluble in cold water.

**Section 10: Stability and Reactivity Data**

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances: Not available.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Not available.
Special Remarks on Corrosivity: Not available.
Polymerization: No.

**Section 11: Toxicological Information**

Routes of Entry: Dermal contact. Eye contact. Inhalation. Ingestion.
Toxicity to Animals:
Acute oral toxicity (LD50): 1400 mg/kg [Rat]. Acute dermal toxicity (LD50): 12300 mg/kg [Rabbit].
Chronic Effects on Humans: The substance is toxic to lungs, the nervous system, mucous membranes.
Other Toxic Effects on Humans: Very hazardous in case of skin contact (irritant, permeator), of ingestion, of inhalation.
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans: Not available.
Special Remarks on other Toxic Effects on Humans: Not available.

**Section 12: Ecological Information**

Ecotoxicity: Not available.
BOD5 and COD: Not available.
Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The products of degradation are more toxic.
Special Remarks on the Products of Biodegradation: Not available.

**Section 13: Disposal Considerations**

Waste Disposal:

**Section 14: Transport Information**

DOT Classification: Class 3: Flammable liquid.
Identification: Isopropylbenzene: UN1918 PG: III
### Section 15: Other Regulatory Information

**Federal and State Regulations:**
- Pennsylvania RTK: Cumene Massachusetts RTK.
- Cumene TSCA 8(b) inventory: Cumene SARA 313 toxic chemical notification and release reporting: Cumene CERCLA: Hazardous substances: Cumene

**Other Regulations:**

**Other Classifications:**
- WHMIS (Canada):
  - CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F).
- DSCL (EEC):
  - R10- Flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes.

**HMIS (U.S.A.):**
- Health Hazard: 2
- Fire Hazard: 3
- Reactivity: 0
- Personal Protection: h

**National Fire Protection Association (U.S.A.):**
- Health: 2
- Flammability: 3
- Reactivity: 1

**Specific hazard:**

**Protective Equipment:**
- Gloves. Lab coat. Respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

### Section 16: Other Information

**References:** Not available.

**Other Special Considerations:** Not available.

**Created:** 10/11/2005 11:43 AM

**Last Updated:** 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Sodium hydroxide, Pellets, Reagent ACS MSDS

Section 1: Chemical Product and Company Identification

| Product Name: Sodium hydroxide, Pellets, Reagent ACS | Contact Information: |
| Catalog Codes: SLS4090 | Sciencelab.com, Inc. |
| CAS#: 1310-73-2 | 14025 Smith Rd. |
| RTECS: W54900000 | Houston, Texas 77396 |
| TSCA: TSCA 8(b) inventory: Sodium hydroxide | US Sales: 1-800-991-7247 |
| Cfl: Not available. | International Sales: 1-281-441-4400 |
| Synonym: Caustic Soda | Order Online: ScienceLab.com |
| Chemical Name: Sodium Hydroxide | CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300 |
| Chemical Formula: NaOH | International CHEMTREC, call: 1-703-527-3887 |
| | For non-emergency assistance, call: 1-281-441-4400 |

Section 2: Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sodium hydroxide</td>
<td>1310-73-2</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Sodium hydroxide LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of skin contact (corrosive, irritant, permeator), of eye contact (irritant, corrosive), of ingestion, of inhalation. The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage.
Section 4: First Aid Measures

**Eye Contact:**
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention immediately.

**Skin Contact:**
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Cover the irritated skin with an emollient. Cold water may be used. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention immediately.

**Serious Skin Contact:**
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

**Inhalation:**
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.

**Serious Inhalation:**
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

**Ingestion:**
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

**Serious Ingestion:** Not available.

Section 5: Fire and Explosion Data

**Flammability of the Product:** Non-flammable.

**Auto-Ignition Temperature:** Not applicable.

**Flash Points:** Not applicable.

**Flammable Limits:** Not applicable.

**Products of Combustion:** Not available.

**Fire Hazards in Presence of Various Substances:**
Of metals

**Explosion Hazards in Presence of Various Substances:**

**Fire Fighting Media and Instructions:** Not applicable.

**Special Remarks on Fire Hazards:**
sodium hydroxide + zinc metal dust causes ignition of the latter. Under proper conditions of temperature, pressure and state of division, it can ignite or react violently with acetaldehyde, ally alcohol, allyl chloride, benzene-1,4-diol, chloro trifluoride, 1,2 dichloroethylene, nitroethane, nitromethane, nitroparaffins, nitropropane, cinnamaldehyde, 2,2-dichloro-3,3-dimethylbutane. Sodium hydroxide in contact with water may generate enough heat to ignite adjacent combustible materials. Phosphorous boiled with NaOH yields mixed phosphines which may ignite spontaneously in air. sodium hydroxide and cinnamaldehyde + heat may cause ignition. Reaction with certain metals releases flammable and explosive hydrogen gas.

**Special Remarks on Explosion Hazards:**
Sodium hydroxide reacts to form explosive products with ammonia + silver nitrate. Benzene extract of allyl benzenesulfonate prepared from allyl alcohol, and benzene sulfonyl chloride in presence of aqueous sodium hydroxide, under vacuum distillation, residue darkened and exploded. Sodium Hydroxide + impure tetrahydrofuran, which can contain peroxides, can
cause serious explosions. Dry mixtures of sodium hydroxide and sodium tetrahydroborate liberate hydrogen explosively at 230-270 deg. C. Sodium Hydroxide reacts with sodium salt of trichlorophenol + methyl alcohol + trichlorobenzene + heat to cause an explosion.

Section 6: Accidental Release Measures

Small Spill:
Use appropriate tools to put the spilled solid in a convenient waste disposal container. If necessary, Neutralize the residue with a dilute solution of acetic acid.

Large Spill:
Corrosive solid. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas, dikes if needed. Call for assistance on disposal. Neutralize the residue with a dilute solution of acetic acid. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep container dry. Do not breathe dust. Never add water to this product. In case of insufficient ventilation, wear suitable respiratory equipment. If you feel unwell, seek medical attention and show the label when possible. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, reducing agents, metals, acids, alkalis, moisture.

Storage: Keep container tightly closed. Keep container in a cool, well-ventilated area. Do not store above 23°C (73.4°F).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient, consult a specialist BEFORE handling this product.

Exposure Limits:
CEIL: 2 from ACGIH (TLV) [United States] [1995] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.
Odor: Odorless.
Taste: Not available.
Molecular Weight: 40 g/mole
Color: White.
PH (1% soln/water): 13.5 [Basic]
Section XII: Appendices

Boiling Point: 1388°C (2530.4°F)
Melting Point: 323°C (613.4°F)
Critical Temperature: Not available.
Specific Gravity: 2.13 (Water = 1)
Vapor Pressure: Not applicable.
Vapor Density: Not available.
Volatile: Not available.
Odor Threshold: Not available.
Water/Oil Dist. Coeff.: Not available.
Ionity in Water: Not available.
Dispersion Properties: See solubility in water.
Solubility: Easily soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Not available.
Incompatibility with various substances:
Highly reactive with metals. Reactive with oxidizing agents, reducing agents, acids, alkalis, moisture.
Corrosivity: Not available.

Special Remarks on Reactivity:
Hygroscopic. Much heat is evolved when solid material is dissolved in water. Therefore cold water and caution must be used for this process. Sodium hydroxide solution and octanol + diocane during a work-up of a reaction mixture of oxime and diobane in tetrahydrofuran is very exothermic, a mild explosion being noted on one occasion. Reactive with water, acids, acid chlorides, strong bases, strong oxidizing agents, strong reducing agents, flammable liquids, organic halogens, metals (i.e. aluminum, tin, zinc), nitromethane, glacial acetic acid, acetic anhydride, acrolein, chlorohydrin, chlorosulfonic acid, ethylene cyanohydrin, glyoxal, hydrochloric acid, sulfuric acid, hydrochloric acid, nitric acid, oleum, propiolactone, acrylonitrile, phosorous pentoxide, chloroethanol, chloroform-methanol, tetrahydroborate, cyanogen azido, 1,2,4,5 tetrachlorobenzene, chininmaldehyde. Reacts with formaldehyde hydroxide to yield formic acid, and hydrogen.

Special Remarks on Corrosivity: Very caustic to aluminum and other metals in presence of moisture.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation. Ingestion.
Toxicity to Animals:
LD50: Not available. LC50: Not available.
Chronic Effects on Humans: Causes damage to the following organs: lungs.
Other Toxic Effects on Humans:
Extremely hazardous in case of inhalation (lung corrosive). Very hazardous in case of skin contact (corrosive, irritant, permeator), of eye contact (corrosive), of ingestion.

Special Remarks on Toxicity to Animals:

p. 4
**Section 12: Ecological Information**

Ecotoxicity: Not available.

BOD5 and COD: Not available.

**Products of Biodegradation:**
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

**Toxicity of the Products of Biodegradation:** The product itself and its products of degradation are not toxic.

**Special Remarks on the Products of Biodegradation:** Not available.

**Section 13: Disposal Considerations**

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

**Section 14: Transport Information**

DOT Classification: Class 8: Corrosive material

Identification: Sodium hydroxide, solid UNNA: 1823 PG II

**Special Provisions for Transport:** Not available.

**Section 16: Other Regulatory Information**

Federal and State Regulations:
Illinois toxic substances disclosure to employee act; Sodium hydroxide Illinois chemical safety act; Sodium hydroxide New York release reporting list; Sodium hydroxide Rhode Island RTK hazardous substances; Sodium hydroxide Pennsylvania RTK; Sodium hydroxide Minnesota; Sodium hydroxide Massachusetts RTK; Sodium hydroxide New Jersey; Sodium hydroxide Louisiana spill reporting; Sodium hydroxide California Director's List of Hazardous Substances; Sodium hydroxide TSCA 8(b) inventory; Sodium hydroxide CERCLA; Hazardous substances: Sodium hydroxide: 1000 lbs. (453.6 kg)

Other Regulations:

Other Classifications:
WHIMIS (Canada): CLASS E: Corrosive solid.
DSCL (EEC):

HMIS (U.S.A.):
   Health Hazard: 3
   Fire Hazard: 0
   Reactivity: 2
   Personal Protection: 

National Fire Protection Association (U.S.A.):
   Health: 3
   Flammability: 0
   Reactivity: 1
   Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

---

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/09/2005 06:32 PM

Last Updated: 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet

Section I. Chemical Product and Company Identification

Chemical Name: 1-Heptene
Catalog Number: H0042
Synonyms: Not available
Chemical Formula: CH₇(CH₂)₆CH₃
CAS Number: 602-76-7
Supplier: TCI America
Address: 3211 N. HarborGate St.
Portland OR 1 800-423-0616

Section II. Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>CAS Number</th>
<th>Percent (%)</th>
<th>TLM/PHEL</th>
<th>Toxicology Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Heptene</td>
<td>602-76-7</td>
<td>Not available</td>
<td>Not available</td>
<td>Not available</td>
</tr>
</tbody>
</table>

Section III. Hazards Identification

Acute Health Effects: Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Inhaling or skin contact. Inhalation causes irritation of the lungs and respiratory system. Inhalation of the eye is characterized by intense, burning, and tearing. Skin irritation is characterized by itching, scaling, retraction, or occasionally, dryness.

Follow site-specific hygiene practices and always wear proper protective equipment when handling this compound.

Chronic Health Effects: CANCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Not available.
Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Section IV. First Aid Measures

Eye Contact: Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.

Skin Contact: In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Inhalation: If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Get medical attention if respiration problems do not improve.

Ingestion: INDUCE VOMITING by slopping fingers in throat. Lower the head so that the vomit will not enter the mouth and throat. Maintain signs clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a positive indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. SEEK IMMEDIATE MEDICAL ATTENTION in case of ingestion of a radioactive material.

Section V. Fire and Explosion Data

Flammability: Flammable
Auto-Ignition: 257 °C (505.0 °F)
Flash Point: -56.9°C (15 °F)
Class: Flammable Limits:
Lower: 1%
Combustible Products:
Those products are toxic carbon oxides (CO, CO₂).
Fire Hazards:
Not available.
Explosion Hazards:
Risks of explosion of the product in presence of mechanical impact: Not available.
Risks of explosion of the product in presence of static discharge: Not available.
Fire Fighting Media:
Flammable liquid.
SMALL FIRE: Use DRY chemical powder.
LARGE FIRE: Use alcohol foam, water spray or fog. Consult with local fire authorities before attempting large scale fire fighting operations.

Continued on Next Page

Emergency phone number: (800) 424-9300
### Section XII: Appendices

#### Section VI. Accidental Release Measures

**Spill Cleanup Instructions:** Flammable liquid. Harmful material. Inhaling material. Keep away from heat. Mechanical exhaust required. Do not use water or dry chemicals. DO NOT touch spilled material. Preserve area, min. sewers, basements or confined areas; dikes if needed. Consult federal, state and local authorities for assistance on disposal.

#### Section VII. Handling and Storage

**Handling and Storage Information:** FLAMMABLE. HARMFUL. IRRITANT. Keep away from heat. Mechanical exhaust required. Avoid excessive heat and light. Do not install in basement. Do not store with incompatible materials. Keep away from heat. DO NOT recap. Do not breathe vapor or use concentrated vapor. Use only with suitable protective clothing. If inhaled, seek medical advice immediately and show the container or the label. Treat symptomatically and supportively. Always store away from incompatible substances such as oxidizing agents.

#### Section VIII. Exposure Controls/Personal Protection

**Engineering Controls:** Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit values. Ensure the exhaust system and safety showers are proximal to the work station location.

**Personal Protection:** Splashes, gloves, lab coat, vapor respirator, boots. Gloves. A MSHAWOSH approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist before handling this product.

**Exposure Limits:** Not available.

#### Section IX. Physical and Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state @ 20°C</td>
<td>Liquid, (Clear, colorless)</td>
</tr>
<tr>
<td>Specific Gravity</td>
<td>0.859 (water=1)</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>88.19</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>94°C (202°F)</td>
</tr>
<tr>
<td>Melting Point</td>
<td>-19°C (-1.6°F)</td>
</tr>
<tr>
<td>Refractive Index</td>
<td>1.504 @ 20°C</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>Not available.</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Not available.</td>
</tr>
<tr>
<td>Solubility</td>
<td>Not available.</td>
</tr>
<tr>
<td>Partition Coefficient</td>
<td>Not available.</td>
</tr>
<tr>
<td>Vapor Pressure</td>
<td>13.6 lb/ft³ (@ 37.7°C)</td>
</tr>
<tr>
<td>Vapor Density</td>
<td>0.7 (Air = 1)</td>
</tr>
<tr>
<td>Volatility</td>
<td>Not available.</td>
</tr>
<tr>
<td>Odor</td>
<td>Not available.</td>
</tr>
<tr>
<td>Taste</td>
<td>Not available.</td>
</tr>
</tbody>
</table>

#### Section X. Stability and Reactivity Data

**Stability:** This material is stable if stored under proper conditions. (See Section VII for instructions)

**Conditions of Instability:** Avoid excessive heat and light.

**Incompatibilities:** Reactive with oxidizing agents.

#### Section XI. Toxicological Information

<table>
<thead>
<tr>
<th>Property</th>
<th>Value/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RTECS Number</td>
<td>Not available.</td>
</tr>
<tr>
<td>Routes of Exposure</td>
<td>Eye Contact, Ingestion, Inhalation.</td>
</tr>
<tr>
<td>Toxicity Data</td>
<td>Not available.</td>
</tr>
<tr>
<td>Chronic Toxic Effects</td>
<td>CANCINOGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td></td>
<td>MUTAGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td></td>
<td>TERATOGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td></td>
<td>DEVELOPMENTAL TOXICITY: Not available.</td>
</tr>
<tr>
<td>Acute Toxic Effects</td>
<td>Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Inhalation causes irritation of the lungs and respiratory system. Irritation of the eyes is characterized by redness, watering, and itching. Skin irritation is characterized by itching, scaling, reddening, or occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.</td>
</tr>
</tbody>
</table>

**Emergency phone number:** (800) 424-9300
Section XII. Ecological Information

- Economic Not available.
- Environmental Fate

1-heptene is expected to have some mobility based on an estimated Koc of 3,500. Volatilization from soil surfaces is expected to be an important fate process based on an estimated Henry's Law constant of 0.427 atm-1 mol-1. 1-heptene may volatilize from dry soil surfaces based on its vapor pressure. 1-heptene's linear hydrocarbon structure would suggest that biodegradation is an important process in soil and water. If released into water, 1-heptene is expected to adsorb to suspended solids and sediment in the water column based on the estimated Koc. Volatilization from water surfaces is expected to be an important fate process based on this compound's Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 3 and 46 hours, respectively. An estimated BCF of 40 suggests the potential for bioconcentration in aquatic organisms is high. Occupational exposure to 1-heptene may occur through inhalation and dermal contact with this compound at workplaces where 1-heptene is produced or used. The general population may be exposed to 1-heptene via inhalation of ambient air.

Section XIII. Disposal Considerations

- Waste Disposal Recycle to process, if possible. Consult your local regulatory authorities. You may be able to dispose of this material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.

Section XIV. Transport Information

- DOT Classification CLASS 5: Flammable liquid.
- UN Number 3427
- Proper Shipping Name 1-Heptene
- Packing Group (PG) I
- DOT Pictograms

Section XV. Other Regulatory Information and Pictograms

- TSCA Chemical Inventory (EPA) This compound is on the EPA Toxic Substances Control Act (TSCA) inventory list.
- WHMIS Classification (Canada) Class A 2: Flammable liquid with a flash point lower than 37.8 °C (100 °F)
- EINECS Number (EEC) 220-767-6
- Japanese Regulatory Data Not available.

Section XVI. Other Information

Version 1.0
Validated on 6/7/2002.

Notice to Reader

TET laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, household or industrial products. The information herein is believed to be correct, but does not claim to be all-inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the responsibility of the user. All chemical names should be handled only by individuals who are familiar with their potential hazards and who have been trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are delineated herein, we cannot guarantee that these are the only hazards which exist. Our SDS sheets are based only on data available at the time of printing and are subject to change without notice as new information is obtained. Avoid long storage periods since the products are subject to degradation with age and may become more hazardous or toxic. If the information in this document is not sufficient, please call or write to the supplier for more information. The product is not intended for human consumption. In the event of accidental release, refer to the emergency procedures provided by the supplier. The supplier is not responsible for the quality or performance of the product. The supplier does not warrant the quality or performance of the product. The supplier makes no representation or warranty regarding the quality or performance of the product. The supplier makes no representation or warranty regarding the quality or performance of the product. The supplier makes no representation or warranty regarding the quality or performance of the product. The supplier makes no representation or warranty regarding the quality or performance of the product.
Material Safety Data Sheet

Section I. Chemical Product and Company Identification

**Chemical Name**
1,2,4-Trimethylbenzene

**Catalog Number**
T0499

**Synonyms**
Pseudocumene

**Chemical Formula**
(CH₃)C₆H₄

**CAS Number**
95-83-8

**Suppliers**
TCI America
9211 N. Harbortage St.
Portland OR
1-800-422-8816

Section II. Composition and Information on Ingredients

<table>
<thead>
<tr>
<th>Chemical Name</th>
<th>CAS Number</th>
<th>Exposure (s)</th>
<th>TLV/PEL</th>
<th>Toxicology Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>95-83-8</td>
<td>Min. 80.0 (GC)</td>
<td>Not available.</td>
<td>Rat LD₅₀ (oral) 6000 mg/kg</td>
</tr>
</tbody>
</table>

Section III. Hazards Identification

**Acute Health Effects**
Harmful if ingested or inhaled. Minimize exposure to this material. Severe overexposure can result in injury or death. Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inhalation of the eye is characterized by redness, watering, and itching. Skin irritation is characterized by itching, scaling, reddening, or occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

**Chronic Health Effects**
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.
DEVELOPMENTAL TOXICITY: Not available.
There is no known effect from chronic exposure to this product. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Section IV. First Aid Measures

**Eye Contact**
Check for and remove any contact lenses. DO NOT use an eye ointment. Flush eyes with running water for a minimum of 15 minutes, occasionally lifting the upper and lower eyelids. Seek medical attention. Treat symptomatically and supportively.

**Skin Contact**
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases, and groin. Cover the irritated skin with an emollient. Seek medical attention. Treat symptomatically and supportively. Wash any contaminated clothing before reusing.

**Inhalation**
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt, or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform artificial respiration. WARNING: It may be dangerous to the person assisting the victim to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious, or corrosive. Seek medical attention. Treat symptomatically and supportively.

**Ingestion**
INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not enter the mouth and throat. Loosen tight clothing such as a collar, tie, belt, or waistband. If the victim is not breathing, administer artificial respiration. Examine the lips and mouth to ascertain whether the tissues are damaged; a possible indication that the toxic material was ingested. Do not attempt to induce vomiting unless instructed to do so by medical personnel. Seek immediate medical attention and, if possible, show the chemical label. Treat symptomatically and supportively.

Section V. Fire and Explosion Data

<table>
<thead>
<tr>
<th>Flammability</th>
<th>Combustible</th>
<th>Auto-Ignition</th>
<th>514°C (957.2°F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flash Point</td>
<td>40°C (104°F)</td>
<td>Flammable Limits</td>
<td>LOWER: 0.9%  UPPER: 5.4%</td>
</tr>
<tr>
<td>Combustion Products</td>
<td>These products are toxic carbon oxides (CO, CO₂)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire Hazard</td>
<td>Flammable in presence of open flames and sparks, or shocks, or heat.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Continued on Next Page

Emergency phone number (800) 424-9300

[Note: The page is a material safety data sheet for a chemical product, providing detailed information on its hazards, first aid measures, and physical properties.]
**Explosion Hazards:**
Risks of explosion of the product in the presence of mechanical impact. Not available.
Risks of explosion of the product in the presence of static discharge. Not available.
No additional information is available regarding the risks of explosion.
- **Small Fire:** Use DRY chemicals. CO₂ water spray or foam.
- **LARGE FIRE:** Use water spray, fog or foam. DO NOT use water jet.

**Section VI. Accidental Release Measures**

**Spill Cleanup Instructions:**
- Combustible material. Harmful material. Irritating material. Keep away from heat and sources of ignition. Mechanical exhaust required. Stop leak if practical. Remove source of ignition. Absorb with DRY earth, sand or other non-combustible material. DO NOT get water inside container. DO NOT touch spilled material. Use water spray to divert vapor drift. Prevent entry into sewers, basements or confined areas. Close exposed areas. Eliminate all sources of ignition. Consult federal, state, and local authorities for assistance on disposal.

**Section VII. Handling and Storage**

**Handling and Storage Information:**
- COMBUSTIBLE. HARMFUL. FRAGILE. Keep away from heat, sources of ignition, and mechanical exhaust required. When not in use, tightly seal the container and store in a cool, dry place.
- Avoid excessive heat and light. DO NOTING. Do not breathe gas, fumes, vapor or spray. In case of insufficient ventilation, wear suitable respiratory equipment.
- If ingested, seek medical advice immediately and show the container or label. Treat symptomatically and supportively.
- Avoid contact with skin and eyes. Always store away from incompatible compounds such as oxidizing agents.

**Section VIII. Exposure Controls/Personal Protection**

**Engineering Controls:**
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash station and safety shower is proximal to the work station location.

**Personal Protection:**
- Splash goggles. Lab coat. Respirator. Boots. Gloves. A NIOSH-approved respirator must be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling the product.

**Exposure Limits:**
Not available.

**Section IX. Physical and Chemical Properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state @ 20°C</td>
<td>Colorless liquid</td>
</tr>
<tr>
<td>Specific Gravity</td>
<td>0.880</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>120.10</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>150°C (302°F)</td>
</tr>
<tr>
<td>Melting Point</td>
<td>44°C (111°F)</td>
</tr>
<tr>
<td>Refractive Index</td>
<td>1.594</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>Not available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Not available</td>
</tr>
</tbody>
</table>

**Solubility:** Soluble in diethyl ether, acetone, polynuclear aromatic hydrocarbons, benzene, ethyl ether. Insoluble in cold water, hot water.

**Partition Coefficient:** Not available.

**Vapor Pressure:** 341 mm Hg (240°C)

**Vapor Density:** Not available.

**Vapor Volume:** Not available.

**Section X. Stability and Reactivity Data**

**Stability:** This material is stable if stored under proper conditions. (See Section VII for instructions)

**Conditions of Instability:** Avoid excessive heat and light.

**Incompatibilities:** Reactive with oxidizing agents.

**Section XI. Toxicological Information**

** RTECS Number:** DOS560000

**Routes of Exposure:**
- Eye contact
- Inhalation
- Ingestion
- Skin contact

**Toxicity Data:**
- Rat LD₅₀ (oral) 5000 mg/kg
- Rabbit LD₅₀ (intraperitoneal) 1785 mg/kg
- Rat LD₅₀ (intraperitoneal) 1785 mg/kg

**Chronic Toxic Effects:**
- CARCINOGENIC EFFECTS: Not available.
- MUTAGENIC EFFECTS: Not available.
- TERATOGENIC EFFECTS: Not available.
- DEVELOPMENTAL TOXICITY: Not available.

There is no known effect from chronic exposure to this product. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

**Continued on Next Page**

**Emergency Phone Number:** (800) 424-9300
Section XII: Ecological Information

Ecotoxicity: Not available.

Environmental Fate: 1,2,4-Trimethylbenzene production and use as an intermediate in the manufacture of trimellitic anhydride, dyestuffs, pharmaceuticals, and pseudocumene may result in its release to the environment through various waste streams. If released to the atmosphere, 1,2,4-trimethylbenzene will exist solely in the vapor phase in the ambient atmosphere, based on a measured vapor pressure of 2.1 mm Hg at 25 deg C. Vapor-phase 1,2,4-trimethylbenzene is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and nitrate radicals with half-lives of about 12 hours and 6-30 days, respectively. An estimated Koc value of 720 suggests that 1,2,4-trimethylbenzene will have low mobility in soil. Volatilization from moist and dry soil surfaces is expected to occur based on a measured Henry's Law constant of 5.1X10^3 atm-mol/m^2. The vapor pressure of this compound, respectively. 1,2,4-trimethylbenzene is expected to adsorb to biologically active sites in both soil and water. Aerosol (polymer microspheres) did not show significant biodegradation in comparison to untreated control. In water, 1,2,4-trimethylbenzene may adsorb to sediment or particulate matter based on its Koc value. This compound is expected to desorb from water surfaces given its Henry's Law constant. Estimated half-lives for a modified bioassay for this compound are 2-4 days, respectively. Biodegradation in aquatic organisms is moderate to high based on BCF values of 31-275. Measured in carp, 1,2,4-trimethylbenzene is expected to photodegrade in natural waters. Occupational exposure may occur through inhalation and dermal contact with this compound at workplaces where it is produced or used. (HODD)

Section XIII: Disposal Considerations

Waste Disposal: Recycle, if possible. Consult local or regional authorities. You may be able to dissolve or mix with a compatible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state, and local regulations when disposing of this substance.

Section XIV: Transport Information

DOT Classification: DOT Class 3: Flammable liquid.

PNI Number: UN1296

Proper Shipping Name: Hydrocarbons liquid, n.o.s.

Packing Group (PG): III

DOT Prohibitions:

Section XV: Other Regulatory Information and Pictograms

TSCA Chemical Inventory (EPA): This compound is ON the EPA Toxic Substances Control Act (TSCA) inventory list.

WHMIS Classification (Canada): WHMIS Class 3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F)

EINECS Number (EEC): 202-430-9

ECC Risk Statements: R12: Flammable. R18: In contact with water, may form flammable/explosive vapor-air mixture. R21/22: Irritating to eyes, respiratory system and skin.

Japanese Regulatory Data: Not available.

Section XVI: Other Information

Version 1.0
Validated on 10/24/1997.

Notice to Reader:

EEC inventory chemicals are for research purposes only and are NOT intended for use to drop, flood, additives, labelable, or possessive. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the manufacturer, supplier nor any of its subsidiaries accept any liability whatsoever for the accuracy or completeness of the information contained herein. Feedback of mistakes or additions is to the sole discretion of the user. All chemical systems must be handled with the recognition that their chemical, physical, and toxicological properties may be beyond the measured or determined. All chemical systems should be handled only by individuals who are familiar with their potential hazards that may be caused by improper label, storage, and chemical handling practices. Although certain hazards are described herein, we can not guarantee that this is the only hazard which exist. Our MTS share is based on data available at the time of shipment and are subject to change without notice as new information is received. Avoid long storage periods since the product is subject to degradation with age and may cause chemical changes or instability. It is the responsibility of the user to review updated MTS data for products that are stored in extended periods. Disposal of unused product must be undertaken in accordance with the rules and regulations that are applicable to the country, state, or local regulations (i.e., aquatic protection, protective clothing, handling equipment, etcetera). For proper handling and disposal, always comply with federal, state, and local regulations.

Printed 3/13/1995
Material Safety Data Sheet

Hydrogen

Section 1. Chemical product and company identification

<table>
<thead>
<tr>
<th>Product name</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supplier</td>
<td>AIRGAS INC., on behalf of its subsidiaries 259 North Radnor-Chester Road Suite 100, Radnor, PA 19087-5263 1-610-687-5253</td>
</tr>
<tr>
<td>Product use</td>
<td>Synthetically/Analytical chemistry.</td>
</tr>
<tr>
<td>Synonym</td>
<td>Dihydrogen; p-Hydrogen; p-Hydrogen; Molecular hydrogen; H2; UN 1049; UN 1668; Liquid hydrogen (LH2 or LH2)</td>
</tr>
<tr>
<td>MSDS #</td>
<td>001026</td>
</tr>
<tr>
<td>Date of Preparation/Revision</td>
<td>4/26/2010</td>
</tr>
<tr>
<td>In case of emergency</td>
<td>1-866-734-3438</td>
</tr>
</tbody>
</table>

Section 2. Hazards identification

<table>
<thead>
<tr>
<th>Physical state</th>
<th>Gas or Liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emergency overview</td>
<td>WARNING! GAS: CONTENTS UNDER PRESSURE. Extremely flammable Do not puncture or incinerate container. Can cause rapid suffocation. May cause severe frostbite.</td>
</tr>
<tr>
<td>Routes of entry</td>
<td>Inhalation</td>
</tr>
<tr>
<td>Potential acute health effects</td>
<td>Eyes: Contact with rapidly expanding gases or liquid can cause frostbite.</td>
</tr>
<tr>
<td></td>
<td>Skin: Contact with rapidly expanding gases or liquid can cause frostbite.</td>
</tr>
<tr>
<td></td>
<td>Inhalation: Acts as a simple asphyxiating agent.</td>
</tr>
<tr>
<td></td>
<td>Ingestion: Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.</td>
</tr>
<tr>
<td>Potential chronic health effects</td>
<td>CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td>Medical conditions aggravated by over-exposure</td>
<td>Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.</td>
</tr>
</tbody>
</table>

See toxicological information (section 11)
Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1333-74-0</td>
<td>100</td>
<td>Oxygen Depletion [Asphyxiant]</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fires are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.
Auto-ignition temperature: 399.85 to 573.75°C (751.7 to 1064.8°F)
Flammable limits: Lower: 4% Upper: 75%
Products of combustion: No specific data.
Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: oxidizing materials.
Fire-fighting media and instructions: Use an extinguishing agent suitable for the surrounding fire.

- Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.
- Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full-face piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.
Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.
Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or crisp. Use a suitable hand truck for cylinder movement.

Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.
### Section 8. Exposure controls/personal protection

**Engineering controls**: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

**Personal protection**

**Eyes**: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

**Skin**: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

**Respiratory**: Use a property fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

**Hands**: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures.

**Personal protection in case of a large spill**

**Product name**: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

**Oxygen Depletion [Asphyxiant]**

Consult local authorities for acceptable exposure limits.

### Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>2.02 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>H2</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>-253.2°C (-423.8°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-259.2°C (-434.6°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>-240.1°C (-400.2°F)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>0.07 (Air = 1)</td>
</tr>
<tr>
<td>Liquid Density@BP: 4.43 lb/ft³ (70.96 kg/m³)</td>
<td></td>
</tr>
<tr>
<td>Specific Volume (ft³/lb)</td>
<td>14.0545</td>
</tr>
<tr>
<td>Gas Density (lb/ft³)</td>
<td>0.071</td>
</tr>
</tbody>
</table>

### Section 10. Stability and reactivity

**Stability and reactivity**: The product is stable.

**Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.

**Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.

**Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.
### Section 11. Toxicological information

**Toxicity data**

- Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.
- Specific effects:
  - Carcinogenic effects: No known significant effects or critical hazards.
  - Mutagenic effects: No known significant effects or critical hazards.
  - Reproduction toxicity: No known significant effects or critical hazards.

### Section 12. Ecological information

**Aquatic ecotoxicity**

- Not available.

**Environmental fate**

- Not available.

**Environmental hazards**

- No known significant effects or critical hazards.

**Toxicity to the environment**

- Not available.

### Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulations. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

### Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1049</td>
<td>HYDROGEN, COMPRESSED</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Limited quantity Yes.</td>
</tr>
<tr>
<td></td>
<td>UN1966</td>
<td>Hydrogen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction Passenger aircraft Quantity limitation: Forbidden. Cargo aircraft Quantity limitation: 150 kg</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1049</td>
<td>HYDROGEN, COMPRESSED</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index 0.125</td>
</tr>
<tr>
<td></td>
<td>UN1966</td>
<td>Hydrogen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>FRAP Index 3000 Passenger Carrying Ship Index Forbidden Passenger</td>
</tr>
</tbody>
</table>
### Section 15. Regulatory Information

**United States**

- **U.S. Federal regulations**
  - TSCA 8(a) IUR: hydrogen
  - United States inventory (TSCA 8b): This material is listed or exempted.
  - SARA 302/304 extremely hazardous substances: No products were found.
  - SARA 302/304 emergency planning and notification: No products were found.
  - SARA 302/304 hazardous chemicals: hydrogen
  - SARA 302/304 hazardous compounds: hydrogen
  - SARA 302/304 risk management plan: hydrogen
  - Clean Water Act (CWA) 307: No products were found.
  - Clean Air Act (CAA) 112 accidental release prevention: hydrogen
  - Clean Air Act (CAA) 112 regulated flammable substances: hydrogen
  - Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

- **State regulations**
  - Connecticut Carcinogen Reporting: This material is not listed.
  - Connecticut Hazardous Materials Survey: This material is not listed.
  - Florida substances: This material is not listed.
  - Illinois Chemical Safety Act: This material is not listed.
  - Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
  - Louisiana Reporting: This material is not listed.
  - Louisiana Spill: This material is not listed.
  - Massachusetts Spill: This material is not listed.
  - Massachusetts Substances: This material is listed.
  - Michigan Critical Material: This material is not listed.
  - Minnesota Hazardous Substances: This material is not listed.
  - New Jersey Hazardous Substances: This material is listed.
  - New Jersey Spill: This material is not listed.
  - New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
  - New York Actively Hazardous Substances: This material is not listed.
  - New York Toxic Chemical Release Reporting: This material is not listed.
  - Pennsylvania RTK Hazardous Substances: This material is listed.
  - Rhode Island Hazardous Substances: This material is not listed.

**Canada**

- **WHMIS (Canada)**
  - Class A: Compressed gas.
  - Class B-1: Flammable gas.
  - CEPA Toxic substances: This material is not listed.
  - Canadian ARET: This material is not listed.
  - Canadian NPRI: This material is not listed.
  - Alberta Designated Substances: This material is not listed.
  - Ontario Designated Substances: This material is not listed.
  - Quebec Designated Substances: This material is not listed.

---

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."
Section 16. Other information

United States
Label requirements: GAS:
- CONTENTS UNDER PRESSURE.
- Extremely flammable
- Do not puncture or incinerate container.
- Can cause rapid suffocation.
- May cause severe frostbite.
LIQUID:
- Extremely flammable
- Extremely cold liquid and gas under pressure.
- Can cause rapid suffocation.
- May cause severe frostbite.

Canada
Label requirements: Class A: Compressed gas.
Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.):
- Health: 0
- Flammability: 4
- Physical hazards: 0
- Liquid:
  - Health: 3
  - Fire hazard: 4
  - Reactivity: 0
  - Personal protection

National Fire Protection Association (U.S.A.):
- Flammability
- Instability
- Special
- Liquid:
  - Health: 3
  - Flammability
  - Instability
  - Special

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
Methane

Section 1. Chemical product and company identification

Product name: Methane
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-877-487-5253
Product use: Synthetic/Analytical chemistry.
Synonym: fire damp; marsh gas; methane (dot); methyl hydride
MSDS #: 001033
Date of Preparation/Revision: 4/25/2016.
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Gas. [COLORLESS GAS; MAY BE A LIQUID UNDER PRESSURE OR REFRIGERATION.]
Emergency overview: WARNING!
---
GAS:
CONTENTS UNDER PRESSURE.
Extremely flammable.
May cause flash fire.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely flammable.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.
Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.
Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry:
Inhalation

Potential acute health effects:
Eyes:
Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Skin:
Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Inhalation:
Acts as a simple asphyxiant.
Ingestion:
Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects:
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure:
Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)
Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>74-82-8</td>
<td>100</td>
<td>ACGIH TLV (United States, 1/2009). TWA: 1000 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.
Auto-ignition temperature: 639.85°C (1183.7°F)
Flash point: Closed cup: -188.15°C (-306.7°F).
Flammable limits: Lower: 5%  Upper: 15%
Products of combustion: Decomposition products may include the following materials: carbon dioxide, carbon monoxide

Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions: In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding areas. If involved in fire, shut off flow immediately if it can be done without risk. Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.
Section 7. Handling and storage

Handling: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

Storage: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

For additional information concerning storage and handling refer to Compressed Gas Association pamphlet P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93.

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill

Product name: methane

ACGIH TLV (United States, 1/2009).
TWA: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.
Section 9. Physical and chemical properties

Molecular weight : 16.05 g/mole
Molecular formula : C-H4
Boiling/condensation point : -161.6°C (-258.9°F)
Melting/freezing point : -182.6°C (-296.7°F)
Critical temperature : -82.4°C (-116.3°F)
Vapor density : 0.55 (Air = 1) Liquid Density@BP: 26.5 lb/ft³ (424.5 kg/m³)
Specific Volume (ft³/lb) : 23.8128
Gas Density (lb/ft³) : 0.04235

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data : No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects
- Carcinogenic effects : No known significant effects or critical hazards.
- Mutagenic effects : No known significant effects or critical hazards.
- Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity : Not available.
Products of degradation : Products of degradation: carbon oxides (CO, CO₂) and water.
Environmental fate : Not available.
Environmental hazards : No known significant effects or critical hazards.
Toxicity to the environment : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1971</td>
<td>Methane, compressed or Methane or Natural gas, compressed (with high methane content)(Methane)</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>UN1972</td>
<td>Methane, refrigerated</td>
<td></td>
<td></td>
<td></td>
<td>-</td>
</tr>
</tbody>
</table>
### Methane

<table>
<thead>
<tr>
<th>TDG Classification</th>
<th>UN1971</th>
<th>(Methane)Methane, compressed or Methane or Natural gas, compressed (with high methane content)</th>
<th>2.1</th>
<th>Not applicable (gas).</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UN1972</td>
<td>Methane, refrigerated liquid</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mexico Classification</th>
<th>UN1971</th>
<th>(Methane)Methane, compressed or Methane or Natural gas, compressed (with high methane content)</th>
<th>2.1</th>
<th>Not applicable (gas).</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UN1972</td>
<td>Methane, refrigerated liquid</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*

## Section 15. Regulatory information

### United States

**U.S. Federal regulations**

- United States Inventory (TSCA 8b): This material is listed or exempted.
  - SARA 302/304/311/312 extremely hazardous substances: No products were found.
  - SARA 302/304 emergency planning and notification: No products were found.
  - SARA 302/304/311/312 hazardous chemicals: methane
- SARA 311/312 MSDS distribution • chemical inventory • hazard identification: methane: Fire hazard, Sudden release of pressure
- Clean Water Act (CWA) 307: No products were found.
- Clean Water Act (CWA) 311: No products were found.
- Clean Air Act (CAA) 112 accidental release prevention: methane
- Clean Air Act (CAA) 112 regulated flammable substances: methane
- Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

### State regulations

- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is not listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
Section XII: Appendices

Methane

New Jersey Hazardous Substances: This material is listed.
New Jersey Spill: This material is not listed.
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
New York Acutely Hazardous Substances: This material is not listed.
New York Toxic Chemical Release Reporting: This material is not listed.
Pennsylvania RTK Hazardous Substances: This material is listed.
Rhode Island Hazardous Substances: This material is not listed.

Canada
WHMIS (Canada)

- Class A: Compressed gas.
- Class B-1: Flammable gas.
- CEPA Toxic substances: This material is listed.
- Canadian ARET: This material is not listed.
- Canadian NPRI: This material is listed.
- Alberta Designated Substances: This material is not listed.
- Ontario Designated Substances: This material is not listed.
- Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States
Label requirements

- GAS: CONTENTS UNDER PRESSURE.
  Extremely flammable.
  May cause flash fire.
  Do not puncture or incinerate container.
  Can cause rapid suffocation.
  May cause severe frostbite.
- LIQUID: Extremely flammable.
  Extremely toxic liquid and gas under pressure.
  Can cause rapid suffocation.
  May cause severe frostbite.

Canada
Label requirements

- Class A: Compressed gas.
- Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.)

<table>
<thead>
<tr>
<th>Category</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>1</td>
</tr>
<tr>
<td>Flammability</td>
<td>4</td>
</tr>
<tr>
<td>Physical hazards</td>
<td>0</td>
</tr>
</tbody>
</table>

Liquid:

<table>
<thead>
<tr>
<th>Category</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>3</td>
</tr>
<tr>
<td>Fire hazard</td>
<td>4</td>
</tr>
<tr>
<td>Reactivity</td>
<td>1</td>
</tr>
<tr>
<td>Personal protection</td>
<td></td>
</tr>
</tbody>
</table>

National Fire Protection Association (U.S.A.)

- Flammability
  - Health < 1
  - Instability 0
  - Special

Page: 67
**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
### Section 1. Chemical product and company identification

<table>
<thead>
<tr>
<th>Product name</th>
<th>Ethane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supplier</td>
<td>AIRGAS INC., on behalf of its subsidiaries 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-697-5253</td>
</tr>
<tr>
<td>Synonym</td>
<td>Bimethyl; Dimethyl; Ethyl hydrate; Methylymethane; C2H6; UN 1035; UN 1961</td>
</tr>
<tr>
<td>MSDS #</td>
<td>001024</td>
</tr>
<tr>
<td>Date of Preparation/Revision</td>
<td>4/26/2010.</td>
</tr>
<tr>
<td>In case of emergency</td>
<td>1-866-734-3438</td>
</tr>
</tbody>
</table>

### Section 2. Hazards identification

**Physical state**: Gas. [COLORLESS LIQUEFIED COMPRESSED GAS WITH A MILD GASOLINE-LIKE ODOR.]

**Emergency overview**: WARNING!
- GAS.
- CONTENTS UNDER PRESSURE.
- Extremely flammable.
- May cause flash fire.
- Do not puncture or incinerate container.
- Can cause rapid suffocation.
- May cause severe frostbite.
- LIQUID:
  - Extremely flammable.
  - Extremely cold liquid and gas under pressure.
  - Can cause rapid suffocation.
  - May cause severe frostbite.
- Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.
- Contact with rapidly expanding gases or liquids can cause frostbite.

**Routes of entry**

**Potential acute health effects**

- Eyes: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
- Skin: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
- Inhalation: Acts as a simple asphyxiant.
- Ingestion: Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

**Potential chronic health effects**

- Carcinogenic effects: Not available.
- Mutagenic effects: Not available.
- Teratogenic effects: Not available.

**Medical conditions aggravated by over-exposure**

- Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

**See toxicological information (section 11)**
Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethene</td>
<td>74-84-0</td>
<td>100</td>
<td>ACGH TLY (United States, 1/2009). TWA: 1000 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

<table>
<thead>
<tr>
<th>Flammability of the product</th>
<th>Flammable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto-ignition temperature</td>
<td>530°C (986°F)</td>
</tr>
<tr>
<td>Flash point</td>
<td>Closed cup: -135.15°C (-211.3°F)</td>
</tr>
<tr>
<td>Flammable limits</td>
<td>Lower: 3%; Upper: 12.5%</td>
</tr>
<tr>
<td>Products of combustion</td>
<td>Decomposition products may include the following materials: carbon dioxide carbon monoxide</td>
</tr>
</tbody>
</table>

Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: oxidizing materials.

Fire-fighting media and instructions: In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.
## Section 7. Handling and storage

**Handling**: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement. Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

**Storage**: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 82 °C (126 °F). For additional information concerning storage and handling refer to Compressed Gas Association pamphlet P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

## Section 8. Exposure controls/personal protection

**Engineering controls**: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

**Personal protection**

- **Eyes**: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. When working with cryogenic liquids, wear a full face shield.

- **Skin**: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

- **Respiratory**: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910.134 and (Canada) 294.4-93.

- **Hands**: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Insulated gloves suitable for low temperatures.

- **Personal protection in case of a large spill**

  **Product name**: ACGIH TLV (United States, 1/2009).
  **ethane**
  **TWA**: 1000 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.
**Section 9. Physical and chemical properties**

- **Molecular weight**: 30.08 g/mole
- **Molecular formula**: C2 H6
- **Boiling/condensation point**: -83.2°C (-126.8°F)
- **Melting/freezing point**: -172.2°C (-276°F)
- **Critical temperature**: 32.4°C (90.3°F)
- **Vapor pressure**: 543 (psig)
- **Vapor density**: 1.1 (Air = 1) Liquid Density: BP@34.1 lb/ft³ (546 kg/m³)
- **Specific Volume (ft³/lb)**: 12.6582
- **Gas Density (lb/ft³)**: 0.079

**Section 10. Stability and reactivity**

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.

**Section 11. Toxicological information**

- **Toxicity data**: No specific information is available in our database regarding the other toxic effects of this material to humans.
- **Specific effects**:
  - **Carcinogenic effects**: No known significant effects or critical hazards.
  - **Mutagenic effects**: No known significant effects or critical hazards.
  - **Reproductive toxicity**: No known significant effects or critical hazards.

**Section 12. Ecological information**

**Aquatic ecotoxicity**

- Not available.

- **Products of degradation**: Products of degradation: carbon oxides (CO, CO2) and water.
- **Environmental fate**: Not available.
- **Environmental hazards**: No known significant effects or critical hazards.
- **Toxicity to the environment**: Not available.

**Section 13. Disposal considerations**

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to AirGas, Inc. Do not dispose of locally.

**Section 14. Transport information**

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DOT Classification</strong></td>
<td>UN1036</td>
<td>ETHANE</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Limited quantity Yes.</td>
</tr>
<tr>
<td></td>
<td>UN1961</td>
<td>Ethane, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction Passenger aircraft</td>
</tr>
</tbody>
</table>
### Section XII: Appendices

#### Ethane

<table>
<thead>
<tr>
<th>TDG Classification</th>
<th>UN1035</th>
<th>UN1961</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ETHANE</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ethane, refrigerated liquid</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mexico Classification</th>
<th>UN1035</th>
<th>UN1961</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ETHANE</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ethane, refrigerated liquid</td>
<td></td>
</tr>
</tbody>
</table>

- **Quantity limitation:** Forbidden.
- **Cargo aircraft Quantity limitation:** 150 kg
- **Explosive Limit and Limited Quantity Index:** 0.125
- **ERAP Index:** 3000
- **Passenger Carrying Ship Index:** Forbidden
- **Passenger Carrying Road or Rail Index:** Forbidden

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*

### Section 15. Regulatory information

**United States**

**U.S. Federal regulations**

- **United States Inventory (TSCA 8b):** This material is listed or exempted.
- **SARA 302/304/311/312 extremely hazardous substances:** No products were found.
- **SARA 302/304 emergency planning and notification:** No products were found.
- **SARA 302/304/311/312 hazardous chemicals:** Ethane
- **SARA 311/313 SDSMS distribution - chemical inventory - hazard identification:** Ethane: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard
- **Clean Water Act (CWA) 307:** No products were found.
- **Clean Water Act (CWA) 311:** No products were found.
- **Clean Air Act (CAA) 112 accidental release prevention:** Ethane
- **Clean Air Act (CAA) 112 regulated flammable substances:** Ethane
- **Clean Air Act (CAA) 112 regulated toxic substances:** No products were found.
### Ethane

**State regulations**
- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Floride substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is not listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is not listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
- New York Acutely Hazardous Substances: This material is not listed.
- New York Toxic Chemical Release Reporting: This material is not listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

**Canada**

**WHMIS (Canada)**
- Class A: Compressed gas.
- Class B-1: Flammable gas.
- CEPA Toxic substances: This material is listed.
- Canadian ARET: This material is not listed.
- Canadian NPRI: This material is listed.
- Alberta Designated Substances: This material is not listed.
- Ontario Designated Substances: This material is not listed.
- Quebec Designated Substances: This material is not listed.

### Section 16. Other information

**United States**

**Label requirements**
- GAS:
  - CONTENTS UNDER PRESSURE.
  - Extremely flammable.
  - May cause flash fire.
  - Do not puncture or incinerate container.
  - Can cause rapid suffocation.
  - May cause severe frostbite.
- LIQUID:
  - Extremely flammable.
  - Extremely cold liquid and gas under pressure.
  - Can cause rapid suffocation.
  - May cause severe frostbite.

**Canada**

**Label requirements**
- Class A: Compressed gas.
- Class B-1: Flammable gas.

**Hazardous Material Information System (U.S.A.)**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Flammability</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Physical hazards</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

**Liquid:**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>3</td>
</tr>
</tbody>
</table>
Ethane

<table>
<thead>
<tr>
<th>Fire hazard</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactivity</td>
<td>0</td>
</tr>
<tr>
<td>Personal protection</td>
<td></td>
</tr>
</tbody>
</table>

National Fire Protection Association (U.S.A.)

Flammability
Health 0 0
Instability
Special

Liquid:

Flammability
Health 3 0
Instability
Special

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

Section 1. Chemical product and company identification

Product name: Propane
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-810-687-5253

Product use: Synthetic/Analytical chemistry.
Synonym: n-Propane; Dimethylmethane; Freon 290; Liquefied petroleum gas; Lpg; Propyl
hydrorida; R 290; C3H8; UN 1075; UN 1078; A-108; Hydrocarbon propellant.
MSDS #: 001045
Date of Preparation/Revision: 4/28/2011.

In case of emergency: 1-866-734-3436

Section 2. Hazards identification

Physical state: Gas. [COLORLESS LIQUEFIED COMPRESSED GAS; ODORLESS BUT MAY HAVE
SKUNK ODO ADDED.]

Emergency overview: WARNING!
FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. May
cause target organ damage, based on animal data. Use only with adequate ventilation.
Keep container closed.
Contact with rapidly expanding gases can cause frostbite.

Target organs: May cause damage to the following organs: the nervous system, heart, central nervous
system (CNS).

Routes of entry:
Inhalation:

Potential acute health effects:
Eyes: Contact with rapidly expanding gas may cause burns or frostbite.

Skin: Contact with rapidly expanding gas may cause burns or frostbite.

Inhalation: Acts as a simple asphyxiant.

Ingestion: Ingestion is not a normal route of exposure for gases

Potential chronic health effects:
Chronic effects: May cause target organ damage, based on animal data.

Target organs: May cause damage to the following organs: the nervous system, heart, central nervous
system (CNS).

Medical conditions aggravated by over-exposure:
Pre-existing disorders involving any target organs mentioned in this MSDS as being at
risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)
Section XII: Appendices

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propane</td>
<td>74-98-6</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>ACGIH TLV (United States, 2/2010).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 ppm 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>NIOSH REL (United States, 6/2009).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1800 mg/m³ 10 hours.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 ppm 10 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>GSHA PEL (United States, 5/2010).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1800 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 ppm 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1800 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

- Flammability of the product: Flammable.
- Auto-ignition temperature: 450°C (842°F)
- Flash point: Closed cup: -104°C (-155.2°F). Open cup: -104°C (-155.2°F).
- Flammable limits: Lower: 2.1% Upper: 9.5%
- Products of combustion: Decomposition products may include the following materials: carbon dioxide, carbon monoxide
- Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.
- Fire-fighting media and instructions: In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill

Product name: Propane

ACGIH TLV (United States, 2/2010).
TWA: 1000 ppm 8 hour(s).
NIOSH REL (United States, 6/2009).
TWA: 1800 mg/m³ 10 hour(s).
OSHA PEL (United States, 6/2010).
TWA: 1800 mg/m³ 8 hour(s).
TWA: 1800 mg/m³ 8 hour(s).

Page: 3/7
Section 9. Physical and chemical properties

Molecular weight : 44.11 g/mole
Molecular formula : C3-H8
Boiling/condensation point : -42°C (-43.6°F)
Melting/freezing point : -189.7°C (-309.5°F)
Critical temperature : 96.6°C (205.9°F)
Vapor pressure : 109 (psig)
Vapor density : 1.6 (Air = 1)
Specific Volume (ft³/lb) : 6.0205
Gas Density (lb/ft³) : 0.116

Section 10. Stability and reactivity

Stability and reactivity : The product is stable.
Incompatibility with various substances : Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data
Product/ingredient name : Propane
Result : LC50 Inhalation Gas.
Species : Rat
Dose : >600000 ppm
Exposure : 15 minutes

IDLH : 2100 ppm
Chronic effects on humans : May cause damage to the following organs: the nervous system, heart, central nervous system (CNS).
Other toxic effects on humans : No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects
Carcinogenic effects : No known significant effects or critical hazards.
Mutagenic effects : No known significant effects or critical hazards.
Reproduction toxicity : No known significant effects or critical hazards.

Section 12. Ecological information

Ecotoxicity
Not available.
Products of degradation : Products of degradation: carbon oxides (CO, CO₂) and water.
Environmental fate : Not available.
Environmental hazards : This product shows a low bioaccumulation potential.
Toxicity to the environment : Not available.
### Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

### Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1978</td>
<td>PROPANE</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td><img src="image" alt="Label" /></td>
<td>Limited quantity Yes. Packaging instruction Passenger aircraft. Quantity limitation: Forbidden. Cargo aircraft Quantity limitation: 150 kg Special provisions 19, T60</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1978</td>
<td>PROPANE</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td><img src="image" alt="Label" /></td>
<td>Explosive Limit and Limited Quantity Index 0.125 ERAP Index 3000 Passenger Carrying Ship Index 65 Passenger Carrying Road or Rail Index Forbidden Special provisions 29, 42</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1978</td>
<td>PROPANE</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td><img src="image" alt="Label" /></td>
<td>-</td>
</tr>
</tbody>
</table>

"Refer to CFR 49 (or authority having jurisdiction) to determine the Information required for shipment of the product."
### Section 15. Regulatory information

#### United States

**U.S. Federal regulations**
- TSCA 8(a) IUR: Partial exemption
- United States inventory (TSCA 8b): This material is listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 302/304/311/312 hazardous chemicals: Propane
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Propane: Fire hazard, Sudden release of pressure
- Clean Air Act (CAA) 112 accidental release prevention - Flammable Substances: Propane

**State regulations**
- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
- New York Acute Hazardous Substances: This material is listed.
- New York Toxic Chemical Release Reporting: This material is not listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

#### Canada

**WHMIS (Canada)**
- Class A: Compressed gas.
- Class B-1: Flammable gas.
- CEPA Toxic substances: This material is not listed.
- Canadian ARET: This material is not listed.
- Canadian NPRI: This material is listed.
- Alberta Designated Substances: This material is not listed.
- Ontario Designated Substances: This material is not listed.
- Quebec Designated Substances: This material is not listed.

### Section 16. Other information

#### United States

**Label requirements**
- FLAMMABLE GAS.
- MAY CAUSE FLASH FIRE.
- MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
- CONTENTS UNDER PRESSURE.

#### Canada

**Label requirements**
- Class A: Compressed gas.
- Class B-1: Flammable gas.
Propane

Hazardous Material Information System (U.S.A.):
- Health: 1
- Flammability: 4
- Physical hazards: 0

National Fire Protection Association (U.S.A.):
- Flammability
- Instability
- Health: 1
- Special: 0

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

N-Butane

Section 1. Chemical product and company identification

Product name: N-Butane
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use: Synthetic/Analytical chemistry.
Synonym: n-Butane; Diethyl; Fracon 600; Liquefied petroleum gas; LPG; n-C4H10; Butan; Butane; Methylthymethane; UN 1011; UN 1075; A-17; Bu-Gas.

MSDS # 001007
Date of Preparation/Revision 11/10/2010.
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Gas. [COLORLESS LIQUEFIED COMPRESS GAS WITH GASOLINE-LIKE ODOR.]
Emergency overview: WARNING!
FLAMMABLE GAS.
MAY CAUSE FLASH FIRE
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.

Keep away from heat, sparks and flame. Do not puncture or incinerate container. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container closed.
Contact with rapidly expanding gases can cause frostbite.

Target organs: May cause damage to the following organs: central nervous system (CNS).
Routes of entry: Inhalation

Potential acute health effects
Eyes: Contact with rapidly expanding gas may cause burns or frostbite.
Skin: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation: Acts as a simple asphyxiant.
Ingestion: Ingestion is not a normal route of exposure for gases

Potential chronic health effects: CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-Butane</td>
<td>109-97-8</td>
<td>100</td>
<td>ACGIH TLV (United States, 2/2010).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 0.1 ppm 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>NIOSH REL (United States, 6/2009).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 mg/m³ 10 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 800 ppm 10 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 1000 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 800 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>
Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.
Auto-ignition temperature: 286.85°C (548.3°F)
Flash point: Closed cup: -60.15°C (-76.3°F).
Flammable limits: Lower: 1.6% Upper: 8.5%
Products of combustion: Decomposition products may include the following materials:
carbon dioxide
carbon monoxide

Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.

Fire-fighting media and instructions: In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 9). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.
**Section 7. Handling and storage**

**Handling**
- Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

**Storage**
- Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

**Section 8. Exposure controls/personal protection**

**Engineering controls**
- Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

**Personal protection**

**Eyes**
- Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

**Skin**
- Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

**Respiratory**
- Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z44.4-93

**Hands**
- Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

**Personal protection in case of a large spill**
- Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

**Product name**
- Butane

**ACGIH TLV (United States, 2/2010).**
- TWA: 1000 ppm 8 hour(s).

**NIOSH REL (United States, 6/2009).**
- TWA: 1900 mg/m³ 10 hour(s).
- TWA: 800 ppm 10 hour(s).

**OSHA PEL 1989 (United States, 3/1989).**
- TWA: 1900 mg/m³ 8 hour(s).
- TWA: 800 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

**Section 9. Physical and chemical properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>58.14 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C4H10</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>-0.6°C (30.9°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-135.4°C (-211.7°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>151.5°C (305.4°F)</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>16.3 (psig)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>2 (Air = 1)</td>
</tr>
</tbody>
</table>
**Section 10. Stability and reactivity**

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.

**Section 11. Toxicological information**

<table>
<thead>
<tr>
<th>Toxicity data</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-Butane</td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>658000 mg/m³</td>
<td>4 hours</td>
</tr>
</tbody>
</table>
| Chronic effects on humans | Vapor | May cause damage to the following organs: central nervous system (CNS).
| Other toxic effects on humans | | No specific information is available in our database regarding the other toxic effects of this material to humans. |

- **Specific effects**
  - **Carcinogenic effects**: No known significant effects or critical hazards.
  - **Mutagenic effects**: No known significant effects or critical hazards.
  - **Reproduction toxicity**: No known significant effects or critical hazards.

**Section 12. Ecological information**

- **Aquatic ecotoxicity**: Not available.
- **Products of degradation**: Products of degradation: carbon oxides (CO, CO₂) and water.
- **Environmental fate**: Not available.
- **Environmental hazards**: No known significant effects or critical hazards.
- **Toxicity to the environment**: Not available.

**Section 13. Disposal considerations**

- Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulations. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

**Section 14. Transport information**

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1011</td>
<td>BUTANE</td>
<td>2.1</td>
<td>Not applicable (gas)</td>
<td></td>
<td>Limited quantity Yes.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation:</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Forbidden.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation:</td>
</tr>
</tbody>
</table>
### Section XII: Appendices

#### N-Butane

<table>
<thead>
<tr>
<th>TDG Classification</th>
<th>UN1011</th>
<th>BUTANE</th>
<th>2.1</th>
<th>Not applicable (gas)</th>
</tr>
</thead>
</table>

- 150 kg
- Special provisions
- 19, T50
- Explosive Limit and Limited Quantity Index
- 0.125
- FRAP Index
- 3000
- Passenger Carrying Ship Index
- Forbidden
- Passenger Carrying Road or Rail Index
- Forbidden
- Special provisions
- 29

*“Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.”*

### Section 15. Regulatory information

**United States**

**U.S. Federal regulations**:
- United States inventory (TSCA 8b): This material is listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 302/304/311/312 hazardous chemicals: Butane
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Butane: Fire hazard, Sudden release of pressure
- Clean Water Act (CWA) 307: No products were found.
- Clean Water Act (CWA) 311: No products were found.
- Clean Air Act (CAA) 112 accidental release prevention: Butane
- Clean Air Act (CAA) 112 regulated flammable substances: Butane
- Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

**State regulations**:
- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.

**Build 1.1**

**Pages: 5/6**
N-Butane

Massachusetts Substances: This material is listed.  
Michigan Critical Material: This material is not listed.  
Minnesota Hazardous Substances: This material is not listed.  
New Jersey Hazardous Substances: This material is listed.  
New Jersey Spill: This material is not listed.  
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.  
New York Acutely Hazardous Substances: This material is not listed.  
New York Toxic Chemical Release Reporting: This material is not listed.  
Pennsylvania RTK Hazardous Substances: This material is listed.  
Rhode Island Hazardous Substances: This material is not listed.

Canada

WHMIS (Canada)
- Class A: Compressed gas.
- Class B-1: Flammable gas.

CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

United States
Label requirements
- FLAMMABLE GAS.
- MAY CAUSE FLASH FIRE.
- MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
- CONTENTS UNDER PRESSURE.

Canada
Label requirements
- Class A: Compressed gas.
- Class B-1: Flammable gas.

Hazardous Material Information System (U.S.A.)
- Health: 1
- Flammability: 4
- Physical hazards: 0

National Fire Protection Association (U.S.A.)
- Flammability: 4
- Health: 1
- Instability: 0
- Special:

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
Pentane and Isomers

Section 1. Chemical product and company identification

Product name: Pentane and Isomers
Supplier: AIRGAS INC., on behalf of its subsidiaries
250 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

MSDS #: 001059
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Liquid.
Emergency overview:
EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. CONTAINS MATERIAL THAT MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Extremely flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. Contains material that may cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.

Target organs: Contains material which may cause damage to the following organs: lungs, upper respiratory tract, skin, eyes, central nervous system (CNS).

Potential acute health effects
Eyes: Irritating to eyes.
Skin: Irritating to skin.
Inhalation: Harmful by inhalation.
Ingestion: No known significant effects or critical hazards.

Potential chronic health effects:
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS Number</th>
<th>VPPM</th>
<th>TWA</th>
</tr>
</thead>
<tbody>
<tr>
<td>isopentane</td>
<td>78-78-4</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>pentane</td>
<td>109-66-0</td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>

Exposure limits
ACGIH TLV (United States, 1/2009).
TWA: 600 ppm 8 hour(s).
ACGIH TLV (United States, 1/2009).
TWA: 600 ppm 8 hour(s).
NIOSH REL (United States, 6/2009).
CEIL: 1800 mg/m³ 15 minute(s).
CEIL: 910 ppm 15 minute(s).
TWA: 350 mg/m³ 10 hour(s).
TWA: 120 ppm 10 hour(s).
OSHA PEL (United States, 11/2006).
TWA: 2500 mg/m³ 8 hour(s).
TWA: 1000 ppm 8 hour(s).
### Section 4. First aid measures

**Eye contact**: Check and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

**Inhalation**: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

### Section 5. Fire-fighting measures

**Flammability of the product**: May be combustible at high temperature.

**Auto-ignition temperature**: Lowest known value: 283.85°C (542.9°F) (pentane).

**Flash point**: Lowest known value: Closed cup: -57.15°C (~70.9°F). (isopentane)

**Flammable limits**: Greatest known range: Lower: 1.4% Upper: 8% (isopentane)

**Products of combustion**: Decomposition products may include the following materials:
- Carbon dioxide
- Carbon monoxide

**Extinguishing media**

**Suitable**: Use dry chemical, CO2, water spray (fog) or foam.

**Not suitable**: Do not use water jet.

**Special exposure hazards**: Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard.

**Special protective equipment for fire-fighters**: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

### Section 6. Accidental release measures

**Personal precautions**: No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).

**Environmental precautions**: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).
Section XII: Appendices

### Section 7. Handling and storage

**Handling**: Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

**Storage**: Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

### Section 8. Exposure controls/personal protection

**Recommended monitoring procedures**: If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

**Engineering measures**: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

**Hygiene measures**: Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reuse. Ensure that eyewash stations and safety showers are close to the workstation location.

**Personal protection**

- **Eyes**: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

- **Skin**: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

- **Respiratory**: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

- **Hands**: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.
**Section 9. Physical and chemical properties**

- **Physical state**: Liquid
- **Boiling/condensation point**: Lowest known value: 27.8°C (82°F) (isopentane). Weighted average: 31.95°C (89.5°F)
- **Melting/freezing point**: May start to solidify at the following temperature: -128.9°C (-200°F) This is based on data for the following ingredient: pentane. Weighted average: -144.7°C (-228.5°F)
- **Critical temperature**: Lowest known value: 187.3°C (369.1°F) (isopentane).
- **Specific gravity**: Weighted average: 0.61 (Water = 1)
- **Vapor density**: Highest known value: 2.5 (Air = 1) (pentane). Weighted average: 2.49 (Air = 1)
- **Evaporation rate**: Highest known value: 12.4 (isopentane) Weighted average: 11.43 compared with butyl acetate
- **VOC**: 100% (w/w)

**Section 10. Stability and reactivity**

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.

**Section 11. Toxicological information**

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>isopentane</td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>290000 mg/m3</td>
<td>4 hours</td>
</tr>
<tr>
<td></td>
<td>LD50 Oral</td>
<td></td>
<td>&gt;2000 mg/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>354 g/m3</td>
<td>4 hours</td>
</tr>
<tr>
<td>pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Chronic effects on humans**: Contains material which may cause damage to the following organs: lungs, upper respiratory tract, skin, eyes, central nervous system (CNS).

**Other toxic effects on humans**: No specific information is available in our database regarding the other toxic effects of this material to humans.

**Specific effects**: No known significant effects or critical hazards.
Section XII: Appendices

**Pentane and Isomors**

**Mutagenic effects**: No known significant effects or critical hazards.

**Reproduction toxicity**: No known significant effects or critical hazards.

**Section 12. Ecological information**

**Aquatic ecotoxicity**

Not available.

**Products of degradation**: Products of degradation: carbon oxides (CO, CO₂) and water.

**Section 13. Disposal considerations**

**Waste disposal**: The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulations. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

**Section 14. Transport information**

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1265</td>
<td>Pentanes, Liquid</td>
<td>3</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1265</td>
<td>Pentanes, Liquid</td>
<td>3</td>
<td>-</td>
<td>Explosive Limit and Limited Quantity Index 0 Passenger Carrying Ship Index Forbidden Passenger Carrying Road or Rail Index 1</td>
<td></td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1265</td>
<td>Pentanes, Liquid</td>
<td>3</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."
### Section 15. Regulatory information

<table>
<thead>
<tr>
<th>United States</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>HCS Classification</strong></td>
</tr>
<tr>
<td>Compressed gas</td>
</tr>
<tr>
<td>Flammable liquid</td>
</tr>
<tr>
<td>Target organ effects</td>
</tr>
<tr>
<td><strong>U.S. Federal regulations</strong></td>
</tr>
<tr>
<td>TSCA 4(a) final test rules: pentane</td>
</tr>
<tr>
<td>TSCA 8(a) PACT: pentane</td>
</tr>
<tr>
<td>United States inventory (TSCA 8b): All components are listed or exempted.</td>
</tr>
<tr>
<td>TSCA 12(b) one-time export: pentane</td>
</tr>
<tr>
<td>SARA 302/304/311/312 extremely hazardous substances: No products were found.</td>
</tr>
<tr>
<td>SARA 302/304 emergency planning and notification: No products were found.</td>
</tr>
<tr>
<td>SARA 302/304/311/312 hazardous chemicals: isopentane; pentane; 2,2-dimethylpropane</td>
</tr>
<tr>
<td>SARA 311/312 MSDS distribution - chemical inventory - hazard identification:</td>
</tr>
<tr>
<td>isopentane: Fire hazard; pentane: Fire hazard, Immediate (acute) health hazard; 2,2-dimethylpropane: Fire hazard, Sudden release of pressure</td>
</tr>
<tr>
<td>Clean Water Act (CWA) 307: No products were found.</td>
</tr>
<tr>
<td>Clean Water Act (CWA) 311: No products were found.</td>
</tr>
<tr>
<td>Clean Air Act (CAA) 112 accidental release prevention: isopentane; pentane; 2,2-dimethylpropane</td>
</tr>
<tr>
<td>Clean Air Act (CAA) 112 regulated flammable substances: isopentane; pentane; 2,2-dimethylpropane</td>
</tr>
<tr>
<td>Clean Air Act (CAA) 112 regulated toxic substances: No products were found.</td>
</tr>
<tr>
<td><strong>State regulations</strong></td>
</tr>
<tr>
<td>Connecticut Carcinogen Reporting: None of the components are listed.</td>
</tr>
<tr>
<td>Connecticut Hazardous Material Survey: None of the components are listed.</td>
</tr>
<tr>
<td>Florida substances: None of the components are listed.</td>
</tr>
<tr>
<td>Illinois Chemical Substances Act: None of the components are listed.</td>
</tr>
<tr>
<td>Illinois Toxic Substances Disclosure to Employee Act: None of the components are listed.</td>
</tr>
<tr>
<td>Louisiana Reporting: None of the components are listed.</td>
</tr>
<tr>
<td>Louisiana Spill: None of the components are listed.</td>
</tr>
<tr>
<td>Massachusetts Spill: None of the components are listed.</td>
</tr>
<tr>
<td>Massachusetts Substances: The following components are listed: ISOPENTANE; PENTANE; 2,2-DIMETHYLPROPANE</td>
</tr>
<tr>
<td>Michigan Critical Material: None of the components are listed.</td>
</tr>
<tr>
<td>Minnesota Hazardous Substances: None of the components are listed.</td>
</tr>
<tr>
<td>New Jersey Hazardous Substances: The following components are listed: ISOPENTANE; BUTANE; 2-METHYL- PENTANE; DIMETHYLPROPANE; 2,2-DIMETHYLPROPANE</td>
</tr>
<tr>
<td>New Jersey Spill: None of the components are listed.</td>
</tr>
<tr>
<td>New Jersey Toxic Catastrophe Prevention Act: None of the components are listed.</td>
</tr>
<tr>
<td>New York Acute Hazardous Substances: None of the components are listed.</td>
</tr>
<tr>
<td>New York Toxic Chemical Release Reporting: None of the components are listed.</td>
</tr>
<tr>
<td>Pennsylvania RTK Hazardous Substances: The following components are listed: BUTANE; 2-METHYL- PENTANE; PROPAINE; 2,2-DIMETHYL-</td>
</tr>
<tr>
<td>Rhode Island Hazardous Substances: None of the components are listed.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Canada</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>WHMIS (Canada)</strong></td>
</tr>
<tr>
<td>Class A: Compressed gas.</td>
</tr>
<tr>
<td>Class B-1: Flammable gas.</td>
</tr>
<tr>
<td>Class B-2: Flammable liquid</td>
</tr>
<tr>
<td><strong>CEPA Toxic substances</strong>: None of the components are listed.</td>
</tr>
<tr>
<td><strong>Canadian ARET</strong>: None of the components are listed.</td>
</tr>
<tr>
<td><strong>Canadian NPRI</strong>: The following components are listed: Pentane; Pentane; Pentane</td>
</tr>
<tr>
<td><strong>Alberta Designated Substances</strong>: None of the components are listed.</td>
</tr>
<tr>
<td><strong>Ontario Designated Substances</strong>: None of the components are listed.</td>
</tr>
<tr>
<td><strong>Quebec Designated Substances</strong>: None of the components are listed.</td>
</tr>
</tbody>
</table>
Section 16. Other information

Label requirements: EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. CONTAINS MATERIAL THAT MAY CAUSE TARGET ORGAN DAMAGE. BASED ON ANIMAL DATA.

Hazardous Material Information System (U.S.A.):
- Health: 1
- Flammability: 4
- Physical hazards: 1

National Fire Protection Association (U.S.A.):
- Health: 1
- Flammability: 0
- Instability: 0
- Special: 0

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.
Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
N-Hexane

Section 1. Chemical product and company identification
Product name: N-Hexane
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-866-887-9253

Synonym: esani (Italian); heksan (Polish); n-hexane; n-hexane; hexane (Dutch); nci-c160571; esani (Italian); heksan (Polish); hexyl hydroxide; normal hexane; hexane (Dutch)
Material uses: Other non-specified industry: SOLVENT, ESPECIALLY FOR VEGETABLE OILS; LOW TEMPERATURE THERMOMETERS; CALIBRATIONS; POLYMERIZATION REACTION MEDIUM; PAINT DILUENT; ALCOHOL DENATURANT.

MSDS #: 001060
Date of Preparation/Revision: 4/27/2010
In case of emergency: 1-866-734-3438

Section 2. Hazards identification
Physical state: Liquid. [COLORLESS LIQUID WITH A MILD GASOLINE-LIKE ODOR]
Emergency overview:
EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA. Extremely flammable liquid. Slightly irritating to the eyes, skin and respiratory system. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use. Wash thoroughly after handling.

Target organs: May cause damage to the following organs: peripheral nervous system, upper respiratory tract, skin, eyes, central nervous system (CNS).

Potential acute health effects:
- Eyes: Slightly irritating to the eyes.
- Skin: Slightly irritating to the skin.
- Inhalation: Slightly irritating to the respiratory system.
- Ingestion: No known significant effects or critical hazards.

Potential chronic health effects:
- CARCINOGENIC EFFECTS: Not available.
- MUTAGENIC EFFECTS: Not available.
- TERATOGENIC EFFECTS: Classified 3 by European Union.

Medical conditions aggravated by over-exposure: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients
United States

Exposure limits
Section XII: Appendices

### N-Hexane

| n-hexane | 110-54-3 | 100 |

ACGIH TLV (United States, 1/2009). Absorbed through skin. TWA: 50 ppm 8 hour(s).

NIOSH REL (United States, 6/2009). TWA: 180 mg/m³ 10 hour(s).

NIOSH REL (United States, 10/2009). TWA: 50 ppm 10 hour(s).

OSHA PEL (United States, 11/2006). TWA: 1800 mg/m³ 8 hour(s).

OSHA PEL (United States, 3/1989). TWA: 180 mg/m³ 8 hour(s).

### Section 4. First aid measures

**Eye contact**: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

**Inhalation**: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

### Section 5. Fire-fighting measures

**Flammability of the product**: Flammable.

**Auto-ignition temperature**: 224.85°C (436.7°F)

**Flash point**: Closed cup: -23.15°C (-9.7°F).

**Flammable limits**: Lower: 1.7% Upper: 7.7%

**Products of combustion**: Decomposition products may include the following materials: carbon dioxide, carbon monoxide

**Fire hazards in the presence of various substances**: Extremely flammable in the presence of the following materials or conditions: oxidizing materials.

**Extinguishing media**: Use dry chemical, CO₂, water spray (fog) or foam.

**Suitable**: Do not use water jet.

**Not suitable**: Promptly isolate the area by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

**Special exposure hazards**: Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

**Special protective equipment for fire-fighters**: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
# N-Hexane

## Section 6. Accidental release measures

**Personal precautions**
- No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No fi res, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).

**Environmental precautions**
- Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

**Methods for cleaning up**
- Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

## Section 7. Handling and storage

**Handling**
- Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

**Storage**
- Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

## Section 8. Exposure controls/personal protection

**Recommended monitoring procedures**
- If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

**Engineering measures**
- Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

**Hygiene measures**
- Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

**Personal protection**
Section XII: Appendices

**N-Hexane**

**Eyes**: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

**Skin**: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

**Respiratory**: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

**Hands**: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

**Personal protection in case of a large spill**

**Product name**

**United States**

**n-hexane**

**Exposure limits**

- **ACGIH TLV (United States, 1/2009).** Absorbed through skin.
  - TWA: 50 ppm 8 hour(s).
  - NIOSH REL (United States, 6/2009).
  - TWA: 180 mg/m³ 10 hour(s).
  - TWA: 50 ppm 10 hour(s).
- **OSHA PEL (United States, 11/2006).**
  - TWA: 1600 mg/m³ 8 hour(s).
  - TWA: 500 ppm 8 hour(s).
- **OSHA PEL 1989 (United States, 3/1989).**
  - TWA: 180 mg/m³ 8 hour(s).
  - TWA: 50 ppm 8 hour(s).

**Section 9. Physical and chemical properties**

- **Physical state**: Liquid. [COLORLESS LIQUID WITH A MILD GASOLINE-LIKE ODOR]
- **Color**: Colorless.
- **Odor**: MILD, GASOLINE-LIKE
- **Molecular weight**: 86.2 g/mole
- **Molecular formula**: C₆H₁₄
- **Boiling/condensation point**: 68.9°C (156°F)
- **Melting/freezing point**: -139.4°C (-218.9°F)
- **Critical temperature**: 234.3°C (453.7°F)
- **Specific gravity**: 0.659 (Water = 1)
- **Vapor density**: 3 (Air = 1)
- **Evaporation rate**: 6.82 compared with butyl acetate
- **VOC**: 0 % (w/w)

**Section 10. Stability and reactivity**

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.
Section 11. Toxicological information

<table>
<thead>
<tr>
<th>Toxicity data</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-hexane</td>
<td>LD50 Oral</td>
<td>Rat</td>
<td>25 g/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LDLo Intraperitoneal</td>
<td>Rat</td>
<td>9100 mg/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>TDL0 Oral</td>
<td>Rat</td>
<td>20000 mg/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Ret</td>
<td>827000 mg/m³</td>
<td>3 minutes</td>
</tr>
<tr>
<td></td>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Ret</td>
<td>96000 ppm</td>
<td>1 hours</td>
</tr>
<tr>
<td></td>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Gas</td>
<td>Ret</td>
<td>49000 ppm</td>
<td>4 hours</td>
</tr>
</tbody>
</table>

IDLH: 1100 ppm

Chronic effects on humans: TERATOGENIC EFFECTS: Classified 3 by European Union. May cause damage to the following organs: peripheral nervous system, upper respiratory tract, skin, eyes, central nervous system (CNS).

Other toxic effects on humans: Hazardous by the following route of exposure: of skin contact (irritant).

Specific effects:
- Carcinogenic effects: No known significant effects or critical hazards.
- Mutagenic effects: No known significant effects or critical hazards.
- Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity

| n-hexane | Acute LC50 113000 μg/L Fresh water | 96 hours |
|          | Mozambique tilapia - Tilapia mossambica - 99 mm - 10 g |       |
|          | Acute LC50 2500 to 2980 μg/L Fresh water | 96 hours |
|          | Fish - Fathead minnow - Pimephales promelas - 31 days - 20.4 mm - 0.123 g |       |

Products of degradation: Products of degradation: carbon oxides (CO, CO₂) and water.

Section 13. Disposal considerations

Waste disposal: The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.
### Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1208</td>
<td>Hexanes (n-hexane)</td>
<td>3</td>
<td>II</td>
<td></td>
<td>Reportable quantity 5000 lbs. (2270 kg)</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1208</td>
<td>Hexanes (n-hexane)</td>
<td>3</td>
<td>II</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index 1 Passenger Carrying Ship Index Forbidden Passenger Carrying Road or Rail Index 5 Reportable quantity 5000 lbs. (2270 kg)</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1208</td>
<td>Hexanes (n-hexane)</td>
<td>3</td>
<td>II</td>
<td></td>
<td>Reportable quantity 5000 lbs. (2270 kg)</td>
</tr>
</tbody>
</table>

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*

### Section 15. Regulatory information

#### United States

**HCS Classification**: Flammable liquid
- Target organ effects

**U.S. Federal regulations**
- United States Inventory (TSCA 8b): This material is listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 311/312 hazardous chemicals: n-hexane
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: n-hexane: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard
- Clean Water Act (CWA) 307: No products were found.
- Clean Water Act (CWA) 311: No products were found.
- Clean Air Act (CAA) 112 accidental release prevention: No products were found.
- Clean Air Act (CAA) 112 regulated flammable substances: No products were found.
- Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

**SARA 313**
- **Product name**:  
- **CAS number**:  
- **Concentration**
<table>
<thead>
<tr>
<th><strong>N-Hexane</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Form R - Reporting requirements</strong></td>
</tr>
<tr>
<td><strong>Supplier notification</strong></td>
</tr>
</tbody>
</table>

SARA 313 notifications must not be detached from the MSDS and any copying and redistribution of the MSDS shall include copying and redistribution of the notice attached to copies of the MSDS subsequently redistributed.

**State regulations**
- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is not listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
- New York Acutely Hazardous Substances: This material is listed.
- New York Toxic Chemical Release Reporting: This material is not listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

**Canada**

**WHMIS (Canada)**
- Class B-2: Flammable liquid
- Class D-2A: Material causing other toxic effects (Very toxic).
- Class D-2B: Material causing other toxic effects (Toxic).
- CEPA Toxic substances: This material is not listed.
- Canadian ARET: This material is not listed.
- Canadian NPRI: This material is listed.
- Alberta Designated Substances: This material is not listed.
- Ontario Designated Substances: This material is not listed.
- Quebec Designated Substances: This material is not listed.

**Section 16. Other information**

**Label requirements**
- EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

**Hazardous Material Information System (U.S.A.)**

**National Fire Protection Association (U.S.A.)**

**Notice to reader**
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
## Material Safety Data Sheet

### n-Heptane

#### Section 1. Chemical product and company identification

- **Product name**: n-Heptane
- **Supplier**: Airgas Inc., on behalf of its subsidiaries
  - 259 North Radnor-Chester Road
  - Suite 100
  - Radnor, PA 19087-5283
  - 1-610-887-5253
- **Synonym**: n-Heptane; Dipropylmethane; Heptyl hydrate; Skellysolve c; n-C7H16; Eplati; Heptan; Heptanen; Getty solving-C; UN 1206; Aliphatic hydrocarbon; Exxsol heptane
- **Material uses**: Other non-specified industry; STANDARD FOR OCTANE RATING DETERMINATIONS (PURE NORMAL HEPTANE HAS ZERO OCTANE NUMBER); ANESTHETIC; SOLVENT; ORGANIC SYNTHESIS; PREPARATION OF LABORATORY REAGENTS.
- **MSDS #**: 001108
- **Date of Preparation/Revision**: 4/28/2010
- **In case of emergency**: 1-866-734-3438

#### Section 2. Hazards identification

- **Physical state**: Liquid. [COLORLESS WATERY LIQUID WITH A GASOLINE-LIKE ODOR]
  - **WARNING**: FLAMMABLE LIQUID AND VAPOR. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
  - Flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.
- **Target organs**: May cause damage to the following organs: upper respiratory tract, skin, central nervous system (CNS).
- **Potential acute health effects**
  - **Eyes**: Irritating to eyes.
  - **Skin**: Irritating to skin.
  - **Inhalation**: IRRITATING TO RESPIRATORY SYSTEM.
  - **Ingestion**: Harmful if swallowed.
- **Potential chronic health effects**: CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available.
- **Medical conditions aggravated by over-exposure**: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

#### Section 3. Composition, Information on Ingredients

**United States**

<table>
<thead>
<tr>
<th>Heptane</th>
<th>142-62-5</th>
<th>100</th>
</tr>
</thead>
</table>

**Exposure limits**

- ACGIH TLV (United States, 1/2009).
  - STEL: 2050 mg/m³ 15 minute(s).
  - STEL: 500 ppm 15 minute(s).
  - TWA: 1640 mg/m³ 8 hour(s).
  - TWA: 400 ppm 8 hour(s).
- NIOSH REL (United States, 6/2009).
  - CEIL: 1600 mg/m³ 15 minute(s).
  - CEIL: 440 ppm 15 minute(s).
Section 4. First aid measures

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.
Auto-ignition temperature: 221.85°C (431.3°F)
Flash point: Closed cup: -4.15°C (24.5°F)
Flammable limits: Lower: 1.1% Upper: 6.7%
Products of combustion: Decomposition products may include the following materials: carbon dioxide, carbon monoxide

Extinguishing media
Suitable: Use dry chemical, CO₂, water spray (fog) or foam.
Not suitable: Do not use water jet.

Special exposure hazards: Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapors are heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flames, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 8).
Section XII: Appendices

**n-Heptane**

**Environmental precautions**: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains, and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

**Methods for cleaning up**: Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact information and section 13 for waste disposal.

### Section 7. Handling and storage

**Handling**: Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, disperse static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

**Storage**: Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully ressealed and kept upright to prevent leakage. Do not store in unsealed containers. Use appropriate containment to avoid environmental contamination.

### Section 8. Exposure controls/personal protection

**Recommended monitoring procedures**: If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

**Engineering measures**: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

**Hygiene measures**: Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

**Personal protection**

**Eyes**: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

**Skin**: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

**Respiratory**: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
### Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>Liquid. [COLORLESS WATERY LIQUID WITH A GASOLINE-LIKE ODOR]</td>
</tr>
<tr>
<td>Odor</td>
<td>GASOLINE</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>100.23 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C7-H16</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>98.3°C (208.9°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-91.1°C (-132°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>266.3°C (512.4°F)</td>
</tr>
<tr>
<td>Specific gravity</td>
<td>0.6836 (Water = 1)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>3.5 (Air = 1)</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>3.18 compared with butyl acetate</td>
</tr>
<tr>
<td>VOC</td>
<td>0 % (w/w)</td>
</tr>
</tbody>
</table>

### Section 10. Stability and reactivity

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.

### Section 11. Toxicological information

<table>
<thead>
<tr>
<th>Toxicity data</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>103 g/m³</td>
<td>4 hours</td>
</tr>
<tr>
<td></td>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>56242 ppm</td>
<td>1 hours</td>
</tr>
<tr>
<td></td>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**IDLH**: 750 ppm
Section XII: Appendices

n-Heptane

Chronic effects on humans: May cause damage to the following organs: upper respiratory tract, skin, central nervous system (CNS).

Other toxic effects on humans: Hazardous by the following route of exposure: of skin contact (irritant).

Specific effects
Carcinogenic effects: No known significant effects or critical hazards.
Mutagenic effects: No known significant effects or critical hazards.
Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity
- Acute LC50 4924000 ug/L Fresh water Fish - Western mosquitofish - Gambusia affinis - Adult 96 hours
- Acute LC50 375000 ug/L Fresh water Fish - Mozambique tilapia - Tilapia mossambica - 99 mm - 10 g 96 hours

Products of degradation: Products of degradation: carbon oxides (CO, CO2) and water.

Section 13. Disposal considerations

Waste disposal: The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional/local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to AirGas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1206</td>
<td>Heptanes</td>
<td>3</td>
<td>II</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1206</td>
<td>Heptanes</td>
<td>3</td>
<td>II</td>
<td>-</td>
<td>Explosive Limit and Limited Quantity Index 1 Passenger Carrying Road or Rail Index 5</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1206</td>
<td>Heptanes</td>
<td>3</td>
<td>II</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
### Section 15. Regulatory information

#### United States

**HCS Classification:** Flammable liquid  
Target organ effects

**U.S. Federal regulations:**  
TSCA 4(a) final test rules: heptane  
TSCA 8(a) PAIR: heptane  
United States inventory (TSCA 8b): This material is listed or exempted.  
TSCA 12(b) one-time export: heptane  
SARA 302/304/311/312 extremely hazardous substances: No products were found.  
SARA 302/304 emergency planning and notification: No products were found.  
SARA 311/312 hazardous chemicals: heptane  
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: heptane: Fire hazard  
Clean Water Act (CWA) 307: No products were found.  
Clean Water Act (CWA) 311: No products were found.  
Clean Air Act (CAA) 112 accidental release prevention: No products were found.  
Clean Air Act (CAA) 112 regulated flammable substances: No products were found.  
Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

#### State regulations

Connecticut Carcinogen Reporting: This material is not listed.  
Connecticut Hazardous Material Survey: This material is not listed.  
Florida substances: This material is not listed.  
Illinois Chemical Safety Act: This material is not listed.  
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.  
Louisiana Reporting: This material is not listed.  
Louisiana Spill: This material is not listed.  
Massachusetts Spill: This material is not listed.  
Massachusetts Substances: This material is listed.  
Michigan Critical Material: This material is not listed.  
Minnesota Hazardous Substances: This material is not listed.  
New Jersey Hazardous Substances: This material is listed.  
New Jersey Spill: This material is not listed.  
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.  
New York Acutely Hazardous Substances: This material is not listed.  
New York Toxic Chemical Release Reporting: This material is not listed.  
Pennsylvania RTK Hazardous Substances: This material is listed.  
Rhode Island Hazardous Substances: This material is not listed.

#### Canada

**WHMIS (Canada):**  
Class B-2: Flammable liquid  
Class D-2B: Motorist causing other toxic effects (Toxic).  
CEPA Toxic substances: This material is not listed.  
Canadian AREG: This material is not listed.  
Canadian NPRE: This material is listed.  
Alberta Designated Substances: This material is not listed.  
Ontario Designated Substances: This material is not listed.  
Quebec Designated Substances: This material is not listed.
### Section 16. Other information

<table>
<thead>
<tr>
<th>Label requirements</th>
<th>Hazardous Material Information System (U.S.A.)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Health</td>
</tr>
<tr>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>National Fire Protection Association (U.S.A.)</th>
<th>Flammability</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Health</td>
</tr>
<tr>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

1-Butene

Section 1. Chemical product and company identification

Product name: 1-Butene
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5223
1-800-927-5253

Product use: Synthetic/Analytical chemistry.

Synonym: n-Butene; 2-Butylene; But-1-ene; Butene-1; Ethylethylene; 1-Butylene; 1-C4H8
MSDS #: 001009

Section 2. Hazards identification

Physical state: Gas. [GAS]

Emergency overview:
WARNING!
FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
CONTENTS UNDER PRESSURE.
Keep away from heat, sparks and flame. Do not puncture or incinerate container. Use only with adequate ventilation. Keep container closed.
Contact with rapidly expanding gases can cause frostbite.

Routes of entry

Potential acute health effects

Eyes: Contact with rapidly expanding gas may cause burns or frostbite.
Skin: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation: Acts as a simple asphyxiant.
Ingestion: Ingestion is not a normal route of exposure for gases

Potential chronic health effects

CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by overexposure

Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

Name: 1-Butene
CAS number: 106-98-9
% Volume: 100
Exposure limits:
ACGIH TLV (United States, 1/2009).
TWA: 250 ppm 8 hour(s).

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.
Section XII: Appendices

1-Butene

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waisband. Get medical attention immediately.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.

Auto-ignition temperature: 384.85°C (724.7°F)

Flammable limits: Lower: 1.6% Upper: 9.3%

Products of combustion: Decomposition products may include the following materials: carbon dioxide, carbon monoxide

Fire-fighting media and instructions: In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).
Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemicals if a risk assessment indicates this is necessary.

Personal protection in case of a large spill

Product name: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight: 56.11 g/mole
Molecular formula: C2H6CH=CH2
Boiling/condensation point: -6.4°C (20.5°F)
Melting/freezing point: -185°C (-301°F)
Critical temperature: 410.4°C (766.9°F)
Vapor pressure: 23.5 (psig)
Vapor density: 1.9 (Air = 1)
Specific Volume (ft³/lb): 6.8965
Gas Density (lb/ft³): 0.145

Section 10. Stability and reactivity

Stability and reactivity: The product is stable.
Incompatibility with various substances: Extremely reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.
Section 11. Toxicological information

Toxicity data
Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects
Carcinogenic effects: No known significant effects or critical hazards.
Mutagenic effects: No known significant effects or critical hazards.
Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity: Not available.
Products of degradation: Products of degradation: carbon oxides (CO, CO₂) and water.
Environmental fate: Not available.
Environmental hazards: No known significant effects or critical hazards.
Toxicity to the environment: Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulations. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1012</td>
<td>Butylene (but-1-ene)</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1012</td>
<td>Butylene (but-1-ene)</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td>Explosive Limit and Limited Quantity Index 0.125 ERAP Index 3000 Passenger Carrying Ship Index Forbidden Passenger Carrying Road or Rail Index Forbidden</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1012</td>
<td>Butylene (but-1-ene)</td>
<td>2.1</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*
## Section 15. Regulatory information

### United States
- **U.S. Federal regulations**
  - **United States inventory (TSCA 8b):** This material is listed or exempted.
  - **SARA 302/304/311/312 extremely hazardous substances:** No products were found.
  - **SARA 302/304 emergency planning and notification:** No products were found.
  - **SARA 302/304/311/312 hazardous chemicals:** No products were found.
  - **SARA 311/312 MSDS distribution - chemical inventory - hazard identification:** No products were found.
  - **Clean Water Act (CWA) 307:** No products were found.
  - **Clean Water Act (CWA) 311:** No products were found.
  - **Clean Air Act (CAA) 112 accidental release prevention:** but-1-ene
  - **Clean Air Act (CAA) 112 regulated flammable substances:** but-1-ene
  - **Clean Air Act (CAA) 112 regulated toxic substances:** No products were found.

### State regulations
- **Connecticut Carcinogen Reporting:** This material is not listed.
- **Florida substances:** This material is not listed.
- **Illinois Chemical Safety Act:** This material is not listed.
- **Illinois Toxic Substances Disclosure to Employee Act:** This material is not listed.
- **Louisiana Reporting:** This material is not listed.
- **Louisiana Spill:** This material is not listed.
- **Massachusetts Spill:** This material is not listed.
- **Massachusetts Substances:** This material is listed.
- **Michigan Critical Material:** This material is not listed.
- **Minnesota Hazardous Substances:** This material is not listed.
- **New Jersey Hazardous Substances:** This material is listed.
- **New Jersey Spill:** This material is not listed.
- **New Jersey Toxic Catastrophe Prevention Act:** This material is not listed.
- **New York Acutely Hazardous Substances:** This material is not listed.
- **New York Toxic Chemical Release Reporting:** This material is not listed.
- **Pennsylvania RTK Hazardous Substances:** This material is listed.
- **Rhode Island Hazardous Substances:** This material is not listed.

### Canada
- **WHMIS (Canada)**
  - **Class A:** Compressed gas.
  - **Class B-1:** Flammable gas.
  - **CEPA Toxic substances:** This material is not listed.
  - **Canadian ARET:** This material is not listed.
  - **Canadian NPRI:** This material is listed.
  - **Alberta Designated Substances:** This material is not listed.
  - **Ontario Designated Substances:** This material is not listed.
  - **Quebec Designated Substances:** This material is not listed.

## Section 16. Other information

### United States
- **Label requirements**
  - **FLAMMABLE GAS.
    MAY CAUSE FLASH FIRE.
    CONTENTS UNDER PRESSURE.

### Canada
- **Label requirements**
  - **Class A:** Compressed gas.
  - **Class B-1:** Flammable gas.
### 1-Butene

<table>
<thead>
<tr>
<th>Hazardous Material Information System (U.S.A.)</th>
<th>National Fire Protection Association (U.S.A.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>Flammability</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>Flammability</td>
<td>Instability</td>
</tr>
<tr>
<td>4</td>
<td>Special</td>
</tr>
<tr>
<td>Physical hazards</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
1-Pentene

Section 1. Chemical product and company identification

<table>
<thead>
<tr>
<th>Product name</th>
<th>1-Pentene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supplier</td>
<td>AIRGAS INC., on behalf of its subsidiaries</td>
</tr>
<tr>
<td></td>
<td>259 North Radnor-Chester Road</td>
</tr>
<tr>
<td></td>
<td>Suite 100</td>
</tr>
<tr>
<td></td>
<td>Radnor, PA 19087-5283</td>
</tr>
<tr>
<td></td>
<td>1-810-867-5253</td>
</tr>
<tr>
<td>Synonym</td>
<td>α-α-Amylene; Propylene; 1-C5H10; Pent-1-ene; 1-Pentene 95; Pentene-1</td>
</tr>
<tr>
<td>MSDS #</td>
<td>001119</td>
</tr>
<tr>
<td>Date of Preparation/Revision</td>
<td>4/28/2010.</td>
</tr>
<tr>
<td>In case of emergency</td>
<td>1-866-734-3438</td>
</tr>
</tbody>
</table>

Section 2. Hazards identification

<table>
<thead>
<tr>
<th>Physical state</th>
<th>Liquid. [COLORLESS LIQUID LIKE GASOLINE]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emergency overview</td>
<td>DANGER!</td>
</tr>
<tr>
<td></td>
<td>EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.</td>
</tr>
<tr>
<td></td>
<td>Extremely flammable liquid. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Target organs</th>
<th>May cause damage to the following organs: skin, eyes, central nervous system (CNS).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potential acute health effects</td>
<td>Eyes: Iritating to eyes.</td>
</tr>
<tr>
<td></td>
<td>Skin: Iritating to skin.</td>
</tr>
<tr>
<td></td>
<td>Inhalation: No known significant effects or critical hazards.</td>
</tr>
<tr>
<td></td>
<td>Ingestion: May be harmful if swallowed.</td>
</tr>
<tr>
<td>Potential chronic health effects</td>
<td>CARCINOGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td></td>
<td>MUTAGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td></td>
<td>TERATOGENIC EFFECTS: Not available.</td>
</tr>
<tr>
<td>Medical conditions aggravated by over-exposure</td>
<td>Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.</td>
</tr>
</tbody>
</table>

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>United States</th>
<th>pent-1-ene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure limits</td>
<td>109-57-1</td>
</tr>
<tr>
<td></td>
<td>100</td>
</tr>
</tbody>
</table>

| Exposure limits     | P О Микдрысць, ПДК (RU, 2/2004), |
|                     | CEIL: 300 mg/m³, (as C) Form: vapor and/or gases |
|                     | TWA: 100 mg/m³, (as C) 8 hour(s). Form: vapor and/or gases |
### Section 4. First aid measures

**Eye contact**: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

**Inhalation**: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

### Section 5. Fire-fighting measures

**Flammability of the product**: Flammable.

**Auto-ignition temperature**: 274.55°C (526.7°F).

**Flash point**: Closed cup: -18.15°C (-0.7°F). Open cup: -18.15°C (-0.7°F).

**Flammable limits**: Lower: 1.4% Upper: 8.7%.

**Products of combustion**: Decomposition products may include the following materials: carbon dioxide, carbon monoxide.

**Fire hazards in the presence of various substances**: Highly flammable in the presence of the following materials or conditions: oxidizing materials.

#### Extinguishing media

**Suitable**: Use dry chemical, CO₂, water spray (fog) or foam.

**Not suitable**: Do not use water jet.

#### Special exposure hazards

Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapors are heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

#### Special protective equipment for fire-fighters

Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

### Section 6. Accidental release measures

#### Personal precautions

No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazardous area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 9).

#### Environmental precautions

Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

#### Methods for cleaning up

Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Container and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact.
### Section 7. Handling and storage

| Handling | Put on appropriate personal protective equipment (see section 6). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container. |
| Storage | Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination. |

### Section 8. Exposure controls/personal protection

| Recommended monitoring procedures | If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment. |
| Engineering measures | Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment. |
| Hygiene measures | Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location. |
| Personal protection | |
| Eyes | Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. |
| Skin | Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. |
| Respiratory | Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. |
| Hands | Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. |
| Personal protection in case of a large spill | Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. |

#### Exposure limits

**United States**

- **PO Минздраг ПДК (RU, 2/2004).**
  - CEIL: 300 mg/m³, (as C) Form: vapor and/or gases
  - TWA: 100 mg/m³, (as C) 8 hour(s), Form: vapor and/or gases
Section 9. Physical and chemical properties

Physical state: Liquid. [COLORLESS LIQUID LIKE GASOLINE]
Color: COLORLESS
Molecular weight: 70.13 g/mole
Molecular formula: C5H10
Boiling/condensation point: 30°C (88°F)
Melting/freezing point: -165.2°C (-265.4°F)
Critical temperature: 191.7°C (377.1°F)
Specific gravity: 0.641 (Water = 1)
Vapor density: 2.4 (Air = 1)
VOC: 0 % (w/w)

Section 10. Stability and reactivity

Stability and reactivity: The product is stable.
Incompatibility with various substances: Highly reactive or incompatible with the following materials: oxidizing materials.
Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Pentene</td>
<td>LC50 Inh</td>
<td>Rat</td>
<td>175000 mg/m³</td>
<td>4 hours</td>
</tr>
<tr>
<td></td>
<td>Vapor</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Chronic effects on humans: May cause damage to the following organs: skin, eyes, central nervous system (CNS).
Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects: No known significant effects or critical hazards.
Mutagenic effects: No known significant effects or critical hazards.
Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity: Not available.

Products of degradation: Products of degradation: carbon oxides (CO, CO₂) and water.

Section 13. Disposal considerations

Waste disposal: The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.
### 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1106</td>
<td>1-PENTENE (N-AMYLENE)</td>
<td>3</td>
<td>i</td>
<td></td>
<td>Limited quantity. Yes.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 1 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 30 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Special provisions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>T11, TP2</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1108</td>
<td>N-AMYLENE; OR 1-PENTENE</td>
<td>3</td>
<td>i</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index 3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger Carrying Ship Index Forbidden</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger Carrying Road or Rail Index 1</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1108</td>
<td>1-PENTENE (N-AMYLENE)</td>
<td>3</td>
<td>i</td>
<td></td>
<td>Limited quantity. Yes.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 1 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 30 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Special provisions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>T11, TP2</td>
</tr>
</tbody>
</table>
Section XII: Appendices

1-Pentene

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*

Section 15. Regulatory information

**United States**

- **HCS Classification**: Flammable liquid
  - Target organ effects
- **U.S. Federal regulations**
  - United States inventory (TSCA 8b): This material is listed or exempted.
  - SARA 302/304 extremely hazardous substances: No products were found.
  - SARA 302/304 emergency planning and notification: No products were found.
  - SARA 302/304/311/312 hazardous chemicals: pent-1-ene
  - SARA 311/312 MSDS distribution - chemical inventory - hazard identification: pent-1-ene; Fire hazard, Immediate (acute) health hazard
  - Clean Water Act (CWA) 307: No products were found.
  - Clean Water Act (CWA) 311: No products were found.
  - Clean Air Act (CAA) 112 accidental release prevention: pent-1-ene
  - Clean Air Act (CAA) 112 regulated flammable substances: pent-1-ene
  - Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

**State regulations**

- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is not listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
- New York Acutely Hazardous Substances: This material is not listed.
- New York Toxic Chemical Release Reporting: This material is not listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

**Canada**

- **WHMIS (Canada)**
  - Class B-2: Flammable liquid
  - CEPA Toxic substances: This material is not listed.
  - Canadian ARET: This material is not listed.
  - Canadian NPI: This material is not listed.
  - Alberta Designated Substances: This material is not listed.
  - Ontario Designated Substances: This material is not listed.
  - Quebec Designated Substances: This material is not listed.

Section 16. Other Information

**Label requirements**

- **Hazardous Material Information System (U.S.A)**
  - Health: 2
  - Flammability: 4
  - Physical hazards: 0

**EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.**
### 1-Pentene

**National Fire Protection Association (U.S.A.)**

<table>
<thead>
<tr>
<th>Flammability</th>
<th>Health</th>
<th>Instability</th>
<th>Special</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

1-Hexene

Section 1. Chemical product and company identification

Product name: 1-Hexene
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5263
1-610-687-5253

Synonym: Hexene-1; 1-n-Hexene; 1-C6H12; Butylethylene; Hexene; Hex-1-ene; UN 2370; Hexylene; Nonene 6

MSDS #: 001067
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Liquid. [COLORLESS LIQUID]
Emergency overview:
DANGER!
EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Extremely flammable liquid. Slightly irritating to the eyes, skin and respiratory system. Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Use only with adequate ventilation. Keep container tightly closed and sealed until ready for use. Wash thoroughly after handling.

Target organs: May cause damage to the following organs: mucous membranes, skin, eyes.

Potential acute health effects:

Eyes: Slightly irritating to the eyes.
Skin: Slightly irritating to the skin.
Inhalation: Slightly irritating to the respiratory system.
Ingestion: No known significant effects or critical hazards.

Potential chronic health effects:
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Not available.

Medical conditions aggravated by over-exposure:
Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)

Section 3. Composition, Information on Ingredients

United States

hex-1-ene: 592-41-6 100

Exposure limits
ACGIH TLV (United States, 1/2009).
TWA: 50 ppm 8 hour(s).
Section 4. First aid measures

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

Inhalation: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

Ingestion: Wash out mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Get medical attention immediately.

Section 5. Fire-fighting measures

Flammability of the product: Flammable.
Auto-ignition temperature: 252.85°C (487.1°F)
Flash point: Closed cup: -9.15°C (15.5°F).
Flammable limits: Lower: 1.2% Upper: 6.9%
Products of combustion: Decomposition products may include the following materials: carbon dioxide, carbon monoxide

Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: oxidizing materials.
Extinguishing media:
Suitable: Use dry chemical, CO₂, water spray (fog) or foam.
Not suitable: Do not use water jet.

Special exposure hazards:
Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. Extremely flammable liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazards.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No fires, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment (see section 9).

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods for cleaning up: Stop leak if without risk. Move containers from spill area. Approach release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillsages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or distomaceous earth and place in container for disposal according to local regulations (see section 13). Use spark-proof tools and explosion-proof equipment. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilled product. Note: see section 1 for emergency contact.
Section XII: Appendices

Section 7. Handling and storage

Handling
Put on appropriate personal protective equipment (see section 8). Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use non-sparking tools. Take precautionary measures against electrostatic discharges. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Empty containers retain product residue and can be hazardous. Do not reuse container.

Storage
Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully ressealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 8. Exposure controls/personal protection

Recommended monitoring procedures
If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment.

Engineering measures
Use with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Hygiene measures
Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking or using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal protection

Eyes
Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin
Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory
Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Hands
Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill

Product name
United States
hex-1-ene

Exposure limits
ACGIH TLV (United States, 1/2009).
TWA: 50 ppm 8 hour(s).
# Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Physical state</th>
<th>Liquid, [COLORLESS LIQUID]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Color</td>
<td>COLORLESS</td>
</tr>
<tr>
<td>Odor</td>
<td>MILD</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>84.18 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C6-H12</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>63°C (145.4°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-98.5°C (-145.3°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>230.3°C (447.6°F)</td>
</tr>
<tr>
<td>Specific gravity</td>
<td>0.6732 (Water = 1)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>3 (Air = 1)</td>
</tr>
<tr>
<td>VOC</td>
<td>0 % (w/w)</td>
</tr>
</tbody>
</table>

# Section 10. Stability and reactivity

<table>
<thead>
<tr>
<th>Stability and reactivity</th>
<th>The product is stable.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Incompatibility with various substances</td>
<td>Extremely reactive or incompatible with the following materials: oxidizing materials.</td>
</tr>
<tr>
<td>Hazardous decomposition products</td>
<td>Under normal conditions of storage and use, hazardous decomposition products should not be produced.</td>
</tr>
<tr>
<td>Hazardous polymerization</td>
<td>Under normal conditions of storage and use, hazardous polymerization will not occur.</td>
</tr>
</tbody>
</table>

# Section 11. Toxicological information

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>hex-1-ene</td>
<td>LD Dermal</td>
<td>Rabbit</td>
<td>&gt;10 g/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LD Oral</td>
<td>Rat</td>
<td>&gt;10 g/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation</td>
<td>Rat</td>
<td>32000 ppm</td>
<td>4 hours, Gas</td>
</tr>
<tr>
<td>Chronic effects on humans</td>
<td>May cause damage to the following organs: mucous membranes, skin, eyes.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other toxic effects on humans</td>
<td>No specific information is available in our database regarding the other toxic effects of this material to humans.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Specific effects</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carcinogenic effects</td>
<td>No known significant effects or critical hazards.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mutagenic effects</td>
<td>No known significant effects or critical hazards.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reproduction toxicity</td>
<td>No known significant effects or critical hazards.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

# Section 12. Ecological information

## Aquatic ecotoxicity

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Acute EC50 60 mg/L</th>
<th>Daphnia - Water</th>
<th>48 hours</th>
</tr>
</thead>
<tbody>
<tr>
<td>hax-1-ene</td>
<td>-</td>
<td>Daphnia magna - &lt;24 hours</td>
<td></td>
</tr>
<tr>
<td>Fresh water</td>
<td>Acute EC50 30 mg/L</td>
<td>Daphnia - Water</td>
<td>48 hours</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>Daphnia magna - &lt;24 hours</td>
<td></td>
</tr>
<tr>
<td>Fresh water</td>
<td>Acute LC50 50 mg/L</td>
<td>Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm</td>
<td>96 hours</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm</td>
<td>96 hours</td>
</tr>
<tr>
<td>Fresh water</td>
<td>Chronic NOEC 32 mg/L</td>
<td>Daphnia - Water</td>
<td>48 hours</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>Daphnia magna - &lt;24 hours</td>
<td></td>
</tr>
</tbody>
</table>
### Section XII: Appendices

**1-Hexene**

- Chronic NOEC 10 mg/L
  - Fresh water
    - magnæ - <24 hours
    - Fish - Zebra danio - Danio rerio - Young - 4 to 6 weeks - 3 cm
    - Daphnia - Water flea - Daphnia magna - <24 hours

**Products of degradation**: Carbon oxides (CO, CO₂) and water.

### Section 13. Disposal considerations

**Waste disposal**: The generation of waste should be avoided or minimized wherever possible. Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe way. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Disposal of this product, solutions, and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

### Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DOT Classification</strong></td>
<td>UN2370</td>
<td>1-HEXENE</td>
<td>3</td>
<td>I</td>
<td></td>
<td>Limited quantity Yes.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger aircraft</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 5 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft Quantity limitation: 60 L</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Special provisions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>I2, T4, TP1</td>
</tr>
<tr>
<td><strong>TDG Classification</strong></td>
<td>UN2370</td>
<td>1-HEXENE</td>
<td>3</td>
<td>I</td>
<td></td>
<td>Passenger Carrying Ship Index</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Forbidden</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger Carrying Road or Rail Index</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5</td>
</tr>
</tbody>
</table>
**1-Hexene**

<table>
<thead>
<tr>
<th>Mexico Classification</th>
<th>UN2370</th>
<th>1-HEXENE</th>
<th>3</th>
<th>II</th>
</tr>
</thead>
</table>

- **Limited quantity**: Yes.
- **Packaging instruction**:
  - Passenger aircraft: Quantity limitation: 5 L
  - Cargo aircraft: Quantity limitation: 60 L
- **Special provisions**: IBC, T4, TP1

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

## Section 15. Regulatory information

### United States

**HCS Classification**:
- Flammable liquid
- Target organ effects

**U.S. Federal regulations**:
- United States inventory (TSCA 8b): This material is listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 302/304/311/312 hazardous chemicals: hex-1-ene
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: hex-1-ene: Fire hazard, Immediate (acute) health hazard
- Clean Water Act (CWA) 307: No products were found.
- Clean Water Act (CWA) 311: No products were found.
- Clean Air Act (CAA) 112 accidental release prevention: No products were found.
- Clean Air Act (CAA) 112 regulated flammable substances: No products were found.
- Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

**Connecticut Carcinogen Reporting**: This material is not listed.
**Connecticut Hazardous Material Survey**: This material is not listed.
**Florida substances**: This material is not listed.
**Illinois Chemical Safety Act**: This material is not listed.
**Illinois Toxic Substances Disclosure to Employee Act**: This material is not listed.
**Louisiana Reporting**: This material is not listed.
**Louisiana Spill**: This material is not listed.
**Massachusetts Spill**: This material is not listed.
**Massachusetts Substances**: This material is listed.
**Michigan Critical Material**: This material is not listed.
**Minnesota Hazardous Substances**: This material is not listed.
**New Jersey Hazardous Substances**: This material is listed.
**New Jersey Spill**: This material is not listed.
**Pennsylvania RTK Hazardous Substances**: This material is listed.
Section XII: Appendices

Section 16. Other information

Label requirements: EXTREMELY FLAMMABLE LIQUID AND VAPOR. FLAMMABLE. VAPOR MAY CAUSE FLASH FIRE. MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION. MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.

Hazardous Material Information System (U.S.A.)
- Health: 1
- Flammability: 3
- Physical hazards: 0

National Fire Protection Association (U.S.A.)
- Flammability
- Health: 1
- Instability: 0
- Special

Notice to reader
To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

1-Hexene

Rhode Island Hazardous Substances: This material is not listed.

Canada
WHIMIS (Canada)
- Class B-2: Flammable liquid
- CEPA Toxic substances: This material is not listed.
- Canadian ARET: This material is not listed.
- Canadian NPRI: This material is listed.
- Alberta Designated Substances: This material is not listed.
- Ontario Designated Substances: This material is not listed.
- Quebec Designated Substances: This material is not listed.
## Material Safety Data Sheet

### Oxygen

**Section 1. Chemical product and company identification**

<table>
<thead>
<tr>
<th><strong>Product name</strong></th>
<th>Oxygen</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Supplier</strong></td>
<td>AIRGAS INC., on behalf of its subsidiaries 258 North Radnor-Chester Road Suite 100 Rednor, PA 19073-5283 1-810-687-5253</td>
</tr>
<tr>
<td><strong>Product use</strong></td>
<td>Synthetic/Analytical chemistry.</td>
</tr>
<tr>
<td><strong>Synonym</strong></td>
<td>Molecular oxygen; Oxygen molecule; Pure oxygen; O2; Liquid-oxygen:- UN 1072; UN 1073; Dioxygen; Oxygen USP, Aviator’s Breathing Oxygen (ABO)</td>
</tr>
<tr>
<td><strong>MSDS #</strong></td>
<td>001043</td>
</tr>
<tr>
<td><strong>Date of Preparation/Revision</strong></td>
<td>6/10/2011</td>
</tr>
<tr>
<td><strong>In case of emergency</strong></td>
<td>1-866-734-3438</td>
</tr>
</tbody>
</table>

**Section 2. Hazards identification**

<table>
<thead>
<tr>
<th><strong>Physical state</strong></th>
<th>Gas.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Emergency overview</strong></td>
<td><strong>DANGER!</strong></td>
</tr>
<tr>
<td></td>
<td>GAS: OXIDIZER. CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE. CONTENTS UNDER PRESSURE. Do not puncture or incinerate container. May cause severe frostbite. LIQUID: OXIDIZER. CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE. Extremely cold liquid and gas under pressure. May cause severe frostbite. Do not puncture or incinerate container. Store in tightly-closed container. Avoid contact with combustible materials. Contact with rapidly expanding gases or liquids can cause frostbite.</td>
</tr>
</tbody>
</table>

**Routes of entry**

**Potential acute health effects**

<table>
<thead>
<tr>
<th><strong>Eyes</strong></th>
<th>May cause eye irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Skin</strong></td>
<td>May cause skin irritation. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.</td>
</tr>
<tr>
<td><strong>Inhalation</strong></td>
<td>Respiratory system irritation after overexposure to high oxygen concentrations.</td>
</tr>
<tr>
<td><strong>Ingestion</strong></td>
<td>Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.</td>
</tr>
<tr>
<td><strong>Medical conditions aggravated by overexposure</strong></td>
<td>Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.</td>
</tr>
</tbody>
</table>

**See toxicological information (Section 11)**
Section XII: Appendices

Oxygen

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxygen</td>
<td>7782-44-7</td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: None expected.

Frostbite: Try to warm up the frozen tissues and seek medical attention.

Inhalation: If inhaled, remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Non-flammable.

Products of combustion: No specific date.

Fire hazards in the presence of various substances: Extremely flammable in the presence of the following materials or conditions: reducing materials, combustible materials and organic materials.

Fire-fighting media and instructions: Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.

Contains gas under pressure. Contact with combustible material may cause fire. This material increases the risk of fire and may aid combustion. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Eliminate all ignition sources if safe to do so. Do not touch or walk through spilled material. Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Notes: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Store in tightly-closed container. Avoid contact with combustible materials. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.
Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection:

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts. When working with cryogenic liquids, wear a full face shield.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator. The applicable standards are (US) 29 CFR 1910 134 and (Canada) Z94.4-93.

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Insulated gloves suitable for low temperatures.

Personal protection in case of a large spill:

Product name: Oxygen

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Molecular weight: 32 g/mole
Molecular formula: O2
Boiling/condensation point: -183°C (-297.4°F)
Melting/freezing point: -218.4°C (-361.1°F)
Critical temperature: -118.6°C (-181.5°F)
Vapor density: 1.105 (Air = 1) Liquid Density@BP: 71.23 lb/ft³ (1141 kg/m³)
Specific Volume (ft³/lb): 12.0462
Gas Density (lb/ft³): 0.083

Section 10. Stability and reactivity

Stability and reactivity: The product is stable.
Incompatibility with various substances: Extremely reactive or incompatible with the following materials: oxidizing materials, reducing materials and combustible materials.
Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.
Section XII: Appendices

Oxygen

Section 11. Toxicological information

Toxicity data
Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects
Carcinogenic effects: No known significant effects or critical hazards.
Mutagenic effects: No known significant effects or critical hazards.
Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity
Not available.
Environmental fate
Not available.
Environmental hazards
This product shows a low bioaccumulation potential.
Toxicity to the environment
Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory Information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1072</td>
<td>OXYGEN, COMPRESSED</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>UN1073</td>
<td>Oxygen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1072</td>
<td>OXYGEN, COMPRESSED</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>UN1073</td>
<td>Oxygen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Section 15. Regulatory Information

**United States**

**U.S. Federal regulations**:
- TSCA 8(a) IUR: Partial exemption
- United States Inventory (TSCA 8(b)): This material is listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 302/304/311/312 hazardous chemicals: Oxygen
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Oxygen: Fire hazard, Sudden release of pressure, Delayed (chronic) health hazard

**State regulations**:
- Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is not listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is not listed.
- New York Acutely Hazardous Substances: This material is not listed.
- New York Toxic Chemical Release Reporting: This material is not listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

**Canada**

**WHMIS (Canada)**:
- Class A: Compressed gas.
- Class C: Oxidizing material.
Section 16. Other information

United States
Label requirements: GAS:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
CONTENTS UNDER PRESSURE.
Do not puncture or incinerate container.
May cause severe frostbite.
LIQUID:
OXIDIZER.
CONTACT WITH COMBUSTIBLE MATERIAL MAY CAUSE FIRE.
Extremely cold liquid and gas under pressure.
May cause severe frostbite.

Canada
Label requirements: Class A: Compressed gas.
Class C: Oxidizing material.

Hazardous Material Information System (U.S.A.):
- Health: 0
- Flammability: 0
- Physical hazards: 0

Liquid:
- Health: 0
- Fire hazard: 0
- Reactivity: 0
- Personal protection: 0

National Fire Protection Association (U.S.A.):
- Health: 0
- Flammability: 0
- Instability: 0
- Special: 0

Liquid:
- Health: 3
- Flammability: 0
- Instability: 0
- Special: 0

Notice to reader
Oxygen

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

Nitrogen

Section 1. Chemical product and company identification

Product name: Nitrogen
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-810-687-5263

Product use: Synthetic/Analytical chemistry. Liquid – cryogenic coolant.

Synonym: nitrogen (colt); nitrogen gas; Nitrogen NF, LIN, Cryogenic Liquid Nitrogen, Liquid Nitrogen

MSDS #: 001040
Date of Preparation/Revision: 1/14/2011.
In case of emergency: 1-866-734-3436

Section 2. Hazards identification

Physical state: Gas. [NORMALLY A COLORLESS GAS. MAY BE A CLEAR COLORLESS LIQUID AT LOW TEMPERATURES. SOLD AS A COMPRESSED GAS OR LIQUID IN STEEL CYLINDERS.]

Emergency overview: WARNING!
GAS:
CONTENTS UNDER PRESSURE.
Do not puncture or incinerate container.
Can cause rapid suffocation.
May cause severe frostbite.
LIQUID:
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.
Do not puncture or incinerate container.
Contact with rapidly expanding gases or liquids can cause frostbite.

Routes of entry
Potential acute health effects

Eyes: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Skin: Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Inhalation: Acts as a simple asphyxiant.

Ingestion: Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Medical conditions aggravated by over-exposure: Acute or chronic respiratory conditions may be aggravated by overexposure to this gas.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>7727-37-9</td>
<td>100</td>
<td>Oxygen Depletion [Asphyxiant]</td>
</tr>
</tbody>
</table>
Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

**Eye contact**: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**: None expected.

**Frostbite**: Try to warm up the frozen tissues and seek medical attention.

**Inhalation**: Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen light clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

**Flammability of the product**: Non-flammable

**Products of combustion**: Decomposition products may include the following materials: nitrogen oxides

**Fire-fighting media and instructions**: Use an extinguishing agent suitable for the surrounding fire.

- Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk.
- Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

**Special protective equipment for fire-fighters**: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

**Personal precautions**: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

**Environmental precautions**: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

**Methods for cleaning up**: Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

**Handling**: High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

- Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

**Storage**: Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.
Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

When working with cryogenic liquids, wear a full face shield.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Insulated gloves suitable for low temperatures

Personal protection in case of a large spill

Product name: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product.

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value/Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>28.02 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>N₂</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>-195.8°C (-320.4°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-210°C (-346°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>-146.9°C (-232.4°F)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>0.967 (Air = 1) Liquid Density@BP: 50.46 lb/ft³ (806.3 kg/m³)</td>
</tr>
<tr>
<td>Specific Volume (ft³/lb)</td>
<td>13.8889</td>
</tr>
<tr>
<td>Gas Density (lb/ft³)</td>
<td>0.072</td>
</tr>
</tbody>
</table>

Section 10. Stability and reactivity

Stability and reactivity: The product is stable.

Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data

Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.

Specific effects

Carcinogenic effects: No known significant effects or critical hazards.

Mutagenic effects: No known significant effects or critical hazards.

Reproduction toxicity: No known significant effects or critical hazards.
Section 12. Ecological information

**Acute ecotoxicity**
Not available.

**Environmental fate** : Not available.
**Environmental hazards** : No known significant effects or critical hazards.
**Toxicity to the environment** : Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory Information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1066</td>
<td>NITROGEN, COMPRESSED</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Limited quantity Yes.</td>
</tr>
<tr>
<td></td>
<td>UN1977</td>
<td>Nitrogen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction Passenger aircraft Quantity limitation: 75 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft Quantity limitation: 150 kg</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1066</td>
<td>NITROGEN, COMPRESSED</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index 0.125</td>
</tr>
<tr>
<td></td>
<td>UN1977</td>
<td>Nitrogen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Passenger Carrying Road or Rail Index 75</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1066</td>
<td>NITROGEN, COMPRESSED</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>UN1977</td>
<td>Nitrogen, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*
**Section 15. Regulatory information**

**United States**

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
</table>
| **U.S. Federal regulations** | TSCA 8(a) IUR: Partial exemption  
United States inventory (TSCA 8b): This material is listed or exempted.  
SARA 302/304/311/312 extremely hazardous substances: No products were found.  
SARA 302/304 emergency planning and notification: No products were found.  
SARA 302/304/311/312 hazardous chemicals: Nitrogen  
SARA 311/312 MSDS distribution - chemical inventory - hazard identification:  
Nitrogen: Sudden release of pressure |

**State regulations**

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
</table>
| Connecticut Carcinogen Reporting: | This material is not listed.  
Connecticut Hazardous Material Survey: This material is not listed.  
Florida substances: This material is not listed.  
Illinois Chemical Safety Act: This material is not listed.  
Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.  
Louisiana Reporting: This material is not listed.  
Louisiana Spill: This material is not listed.  
Massachusetts Spill: This material is not listed.  
Massachusetts Substances: This material is listed.  
Michigan Critical Material: This material is not listed.  
Minnesota Hazardous Substances: This material is not listed.  
New Jersey Hazardous Substances: This material is listed.  
New Jersey Spill: This material is not listed.  
New Jersey Toxic Catastrophe Prevention Act: This material is not listed.  
New York Acutely Hazardous Substances: This material is not listed.  
New York Toxic Chemical Release Reporting: This material is not listed.  
Pennsylvania RTK Hazardous Substances: This material is listed.  
Rhode Island Hazardous Substances: This material is not listed. |

**Canada**

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
</table>
| WHMIS (Canada) | Class A: Compressed gas.  
CEPA Toxic substances: This material is not listed.  
Canadian ARET: This material is not listed.  
Canadian NPI: This material is not listed.  
Alberta Designated Substances: This material is not listed.  
Ontario Designated Substances: This material is not listed.  
Quebec Designated Substances: This material is not listed. |

**Section 16. Other information**

**United States**

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
</table>
| **Label requirements** | GAS:  
CONTENTS UNDER PRESSURE.  
Do not puncture or incinerate container.  
Can cause rapid suffocation.  
May cause severe frostbite.  
LIQUID:  
Extremely cold liquid and gas under pressure.  
Can cause rapid suffocation.  
May cause severe frostbite. |

**Canada**

<table>
<thead>
<tr>
<th>Item</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Label requirements</strong></td>
<td>Class A: Compressed gas.</td>
</tr>
</tbody>
</table>
Nitrogen

**Hazardous Material Information System (U.S.A.)**

- Health: 0
- Flammability: 0
- Physical hazards: 0

**Liquid:**

- Health: 3
- Fire hazard: 0
- Reactivity: 0
- Personal protection: 0

**National Fire Protection Association (U.S.A.)**

- Flammability
  - Health: 0
  - Instability: 0
  - Special: 0

- Liquid:
  - Health: 3
  - Flammability: 0
  - Instability: 0
  - Special: 0

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

Air

Section 1. Chemical product and company identification

Product name: Air
Supplier: AIRGAS INC., on behalf of its subsidiaries
260 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-687-5253

Product use: Synthetic/Analytical chemistry.
Synonym: Compressed Air; Breathing Quality Air; synthetic air, reconstituted air, medical air,
medical air USP.
MSDS #: 001002
Date of Preparation/Revision: 9/9/2011.
In case of emergency: 1-866-734-3436

Section 2. Hazards identification

Physical state: Gas.
Emergency overview: WARNING!
CONTENTS UNDER PRESSURE MAY ACCELERATE COMBUSTION.
COMPRESSED AIR IS A COLORLESS, ODORLESS, TASTELESS GAS AT NORMAL
TEMPERATURE AND PRESSURE.
Do not puncture or incinerate container.
Contact with rapidly expanding gases can cause frostbite.

Target organs: Contains material which may cause damage to the following organs: lungs.

Routes of entry: Inhalation

Potential acute health effects:
Eyes: Contact with rapidly expanding gas may cause burns or frostbite.
Skin: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation: "None expected"
Ingestion: Ingestion is not a normal route of exposure for gases

Potential chronic health effects:
Chronic effects: Contains material that may cause target organ damage, based on animal data.
Target organs: Contains material which may cause damage to the following organs: lungs.

Medical conditions aggravated by over-exposure: None known.

See toxicological information (Section 11)

Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>7727-37-9</td>
<td>76.5 - 80.5</td>
<td>Oxygen Depletion [Asphyxiant]</td>
</tr>
<tr>
<td>Oxygen</td>
<td>7782-44-7</td>
<td>19.5 - 23.5</td>
<td></td>
</tr>
</tbody>
</table>
Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

Eye contact: Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

Skin contact: None expected.

Inhalation: Try to warm up the frozen tissues and seek medical attention.

Ingestion: As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

Flammability of the product: Non-flammable.

Products of combustion: Decomposition products may include the following materials: nitrogen oxides.

Fire-fighting media and instructions: Use an extinguishing agent suitable for the surrounding fire.

Special protective equipment for fire-fighters: Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Keep personnel away. Discard any product, residue, disposable container, or liner in an environmentally acceptable manner, in full compliance with federal, state, and local regulations.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage: Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls: Not applicable

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
Section XII: Appendices

Air

Respiratory: No special protection is required. However, air supplied respirators are required while working in oxygen deficient atmospheres such as confined spaces. The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93.

Hands: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Oxygen Depletion [Asphyxiant]

Consult local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

Boiling/condensation point: -194.3°C (-317.7°F)
Melting/freezing point: -216.2°C (-357.2°F)
Critical temperature: Lowest known value: -146.9°C (-232.4°F) (nitrogen).
Vapor density: Highest known value: 1.1 (Air = 1) (oxygen). Weighted average 1 (Air = 1)
Gas Density (lb/ft³): 0.0749

Section 10. Stability and reactivity

Stability and reactivity: The product is stable.
Incompatibility with various substances: Not considered to be reactive according to our database.
Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Toxicity data
Chronic effects on humans: None known.
Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.
Specific effects
Carcinogenic effects: No known significant effects or critical hazards.
Mutagenic effects: No known significant effects or critical hazards.
Reproduction toxicity: No known significant effects or critical hazards.

Section 12. Ecological information

Aquatic ecotoxicity
Not available.
Products of degradation: Products of degradation: nitrogen oxides (NO, NO₂ etc.).
Environmental fate: Not available.
Environmental hazards: No known significant effects or critical hazards.
Toxicity to the environment: Not available.
Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory Information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1002</td>
<td>Air, compressed</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1002</td>
<td>Air, compressed</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td>Explosive Limit and Limited Quantity Index 0.125 Passenger Carrying Road or Rail Index 75</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1002</td>
<td>Air, compressed</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

"Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product."

Section 15. Regulatory information

United States

U.S. Federal regulations

- TSCA 8(a) IUR: All components are listed or exempted.
- United States inventory (TSCA 8(b)): All components are listed or exempted.
- SARA 302/304/311/312 extremely hazardous substances: No products were found.
- SARA 302/304 emergency planning and notification: No products were found.
- SARA 302/304/311/312 hazardous chemicals: nitrogen; oxygen
- SARA 311/312 MSDS distribution - chemical inventory - hazard identification: nitrogen: Sudden release of pressure; oxygen: Fire hazard; Sudden release of pressure; Delayed (chronic) health hazard

State regulations

- Connecticut Carcinogen Reporting: None of the components are listed.
- Connecticut Hazardous Material Survey: None of the components are listed.
- Florida substances: None of the components are listed.
- Illinois Chemical Safety Act: None of the components are listed.
- Illinois Toxic Substances Disclosure to Employees Act: None of the components are listed.
- Louisiana Reporting: None of the components are listed.
- Louisiana Spill: None of the components are listed.
- Massachusetts Spill: None of the components are listed.
- Massachusetts Substances: The following components are listed: NITROGEN; OXYGEN (LIQUID)
- Michigan Critical Material: None of the components are listed.
- Minnesota Hazardous Substances: None of the components are listed.
- New Jersey Hazardous Substances: The following components are listed: NITROGEN; OXYGEN
Section XIII: Appendices

Air

- New Jersey Spill: None of the components are listed.
- New Jersey Toxic Catastrophe Prevention Act: None of the components are listed.
- New York Acutely Hazardous Substances: None of the components are listed.
- New York Toxic Chemical Release Reporting: None of the components are listed.
- Pennsylvania RTK Hazardous Substances: The following components are listed:
  - NITROGEN; OXYGEN
  - Rhode Island Hazardous Substances: None of the components are listed.

Canada

- WHMIS (Canada): Class A: Compressed gas.
  - CEPA Toxic substances: None of the components are listed.
  - Canadian ARET: None of the components are listed.
  - Canadian NPRI: None of the components are listed.
  - Alberta Designated Substances: None of the components are listed.
  - Ontario Designated Substances: None of the components are listed.
  - Quebec Designated Substances: None of the components are listed.

Section 16. Other information

United States

- Label requirements: CONTENTS UNDER PRESSURE, MAY ACCELERATE COMBUSTION. COMPRessed AIR IS A COLORLESS, ODORLESS, TASTELESS GAS AT NORMAL TEMPERATURE AND PRESSURE.

Canada

- Label requirements: Class A: Compressed gas.

Hazardous Material Information System (U.S.A.)

<table>
<thead>
<tr>
<th>Category</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>0</td>
</tr>
<tr>
<td>Flammability</td>
<td>0</td>
</tr>
<tr>
<td>Physical hazards</td>
<td>0</td>
</tr>
</tbody>
</table>

National Fire Protection Association (U.S.A.)

- Health: 0
- Flammability: 0
- Instability: 0
- Special: 0

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet

Carbon Dioxide

Section 1. Chemical product and company identification

Product name: Carbon Dioxide
Supplier: AIRGAS INC., on behalf of its subsidiaries
259 North Radnor-Chester Road
Suite 100
Radnor, PA 19087-5283
1-610-887-5253

Product use: Synthetic/Analytical chemistry.
Synonym: Carbonic Acid, Carbon Dioxide Liquid, Carbon Dioxide, Refrigerated Liquid, Carbonic Anhydride
MSDS #: 001013
Date of Preparation/Revision: 1/29/2012.
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Gas or Liquid.
Emergency overview: WARNING!
GAS:
CONTENTS UNDER PRESSURE.
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Do not puncture or incinerate container.
Can cause rapid suffocation.

LIQUID:
MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.
CAN CAUSE TARGET ORGAN DAMAGE.
Extremely cold liquid and gas under pressure.
Can cause rapid suffocation.
May cause severe frostbite.

Do not puncture or incinerate container. Avoid contact with eyes, skin and clothing. May cause target organ damage, based on animal data. Wash thoroughly after handling. Keep container closed. Avoid breathing gas. Use with adequate ventilation. Contact with rapidly expanding gas, liquid, or solid can cause frostbite.

Target organs: May cause damage to the following organs: lungs.
Routes of entry: Inhalation Dermal Eyes

Potential acute health effects
Eyes: Moderately irritating to eyes. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Skin: Moderately irritating to the skin. Contact with rapidly expanding gas may cause burns or frostbite. Contact with cryogenic liquid can cause frostbite and cryogenic burns.
Inhalation: Moderately irritating to the respiratory system.
Ingestion: Ingestion is not a normal route of exposure for gases. Contact with cryogenic liquid can cause frostbite and cryogenic burns.

Potential chronic health effects
Chronic effects: May cause target organ damage, based on animal data.
Target organs: May cause damage to the following organs: lungs.

Medical conditions aggravated by over-exposure: Pre-existing disorders involving any target organs mentioned in this MSDS as being at risk may be aggravated by over-exposure to this product.

See toxicological information (Section 11)
Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon Dioxide</td>
<td>124-38-9</td>
<td>100</td>
<td>ACGIH TLV (United States, 2/2010), STEL: 54000 mg/m³ 15 minute(s), STEL: 30000 ppm 15 minute(s), TWA: 9000 mg/m³ 8 hour(s), TWA: 5000 ppm 8 hour(s), NIOSH REL (United States, 6/2009), STEL: 54000 mg/m³ 15 minute(s), STEL: 30000 ppm 15 minute(s), TWA: 9000 mg/m³ 10 hour(s), TWA: 5000 ppm 10 hour(s), OSHA PEL (United States, 6/2010), STEL: 9000 mg/m³ 8 hour(s), TWA: 5000 ppm 8 hour(s), OSHA PEL 1989 (United States, 3/1989), STEL: 30000 ppm 15 minute(s), STEL: 30000 ppm 15 minute(s), TWA: 18000 mg/m³ 8 hour(s), TWA: 10000 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

**Eye contact**
Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**
In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

**Frostbite**
Try to warm up the frozen tissues and seek medical attention.

**Inhalation**
Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**
As this product is a gas, refer to the inhalation section.

Section 5. Fire-fighting measures

**Flammability of the product**
Non-flammable.

**Products of combustion**
Decomposition products may include the following materials: carbon dioxide, carbon monoxide.

**Fire-fighting media and instructions**
Use an extinguishing agent suitable for the surrounding fire.

Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk. Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

**Special protective equipment for fire-fighters**
Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full-facepiece operated in positive pressure mode.
## Carbon Dioxide

### Section 6. Accidental release measures

<table>
<thead>
<tr>
<th>Personal precautions</th>
<th>Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Environmental precautions</td>
<td>Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.</td>
</tr>
<tr>
<td>Methods for cleaning up</td>
<td>Immediately contact emergency personnel. Stop leak if without risk. Note: see section 1 for emergency contact information and section 13 for waste disposal.</td>
</tr>
</tbody>
</table>

### Section 7. Handling and storage

**Handling**
- Wash thoroughly after handling. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Avoid contact with skin and clothing. Use with adequate ventilation. Avoid contact with eyes. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.
- Never allow any unprotected part of the body to touch uninsulated pipes or vessels that contain cryogenic liquids. Prevent entrapment of liquid in closed systems or piping without pressure relief devices. Some materials may become brittle at low temperatures and will easily fracture.

**Storage**
- Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). For additional information concerning storage and handling refer to Compressed Gas Association pamphlets P-1 Safe Handling of Compressed Gases in Containers and P-12 Safe Handling of Cryogenic Liquids available from the Compressed Gas Association, Inc.

### Section 8. Exposure controls/personal protection

**Engineering controls**
- Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits.

**Personal protection**

**Eyes**
- Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.
- When working with cryogenic liquids, wear a full face shield.

**Skin**
- Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

**Respiratory**
- Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
- The applicable standards are (US) 29 CFR 1910.134 and (Canada) Z94.4-93

**Hands**
- Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.
- Insulated gloves suitable for low temperatures

**Personal protection in case of a large spill**
- Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

**Product name**

Build 1.1
Carbon Dioxide

Carbon dioxide

ACGIH TLV (United States, 2/2019).
STEL: 54000 mg/m³ 15 minute(s).
STEL: 3000 ppm 15 minute(s).
TWA: 9000 mg/m³ 8 hour(s).
TWA: 5000 ppm 8 hour(s).

NIOSH REL (United States, 6/2009).
STEL: 54000 mg/m³ 15 minute(s).
STEL: 30000 ppm 15 minute(s).
TWA: 9000 mg/m³ 10 hour(s).
TWA: 5000 ppm 10 hour(s).

OSHA PEL (United States, 6/2010).
TWA: 9000 mg/m³ 8 hour(s).
TWA: 5000 ppm 8 hour(s).

Consent local authorities for acceptable exposure limits.

Section 9. Physical and chemical properties

- Molecular weight: 44.01 g/mole
- Molecular formula: C\textsubscript{2}H\textsubscript{2}
- Melting/freezing point: Sublimation temperature: -79°C (-110.2 to °F)
- Critical temperature: 30.9°C (87.6°F)
- Vapor pressure: 630 (psig)
- Vapor density: 1.53 (Air = 1) Liquid Density@BP: Solid density = 97.5 lb/ft³ (1562 kg/m³)
- Specific Volume (ft\textsuperscript{3}/lb): 8.7719
- Gas Density (lb/ft\textsuperscript{3}): 0.114

Section 10. Stability and reactivity

- Stability and reactivity: The product is stable.
- Hazardous decomposition products: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- Hazardous polymerization: Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

- Toxicity data
  - Product/ingredient name: Carbon dioxide
  - Result: LC50 Inhalation Gas.
  - Species: Rat
  - Dose: 470000 ppm
  - Exposure: 30 minutes

- IDLH: 40000 ppm

- Chronic effects on humans: May cause damage to the following organs: lungs.
- Other toxic effects on humans: No specific information is available in our database regarding the other toxic effects of this material to humans.

- Specific effects
  - Carcinogenic effects: No known significant effects or critical hazards.
  - Mutagenic effects: No known significant effects or critical hazards.
  - Reproduction toxicity: No known significant effects or critical hazards.
**Section 12. Ecological information**

Aquatic ecotoxicity: Not available.
Toxicity of the products of biodegradation: Not available.
Environmental fate: Not available.
Environmental hazards: This product shows a low bioaccumulation potential.
Toxicity to the environment: Not available.

**Section 13. Disposal considerations**

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulations. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

**Section 14. Transport information**

<table>
<thead>
<tr>
<th>Regulatory information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1013</td>
<td>CARBON DIOXIDE</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Limited quantity. Yes.</td>
</tr>
<tr>
<td></td>
<td>UN2187</td>
<td>Carbon dioxide, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Packaging instruction.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Passenger aircraft.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Quantity limitation: 75 kg</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cargo aircraft. Quantity limitation: 150 kg</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1013</td>
<td>CARBON DIOXIDE</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index. 0.126</td>
</tr>
<tr>
<td></td>
<td>UN2187</td>
<td>Carbon dioxide, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td>Passenger Carrying Road or Rail Index. 75</td>
</tr>
<tr>
<td>Mexico Classification</td>
<td>UN1013</td>
<td>CARBON DIOXIDE</td>
<td>2.2</td>
<td>Not applicable (gas).</td>
<td></td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>UN2187</td>
<td>Carbon dioxide, refrigerated liquid</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.*
### Section 15. Regulatory information

#### United States

<table>
<thead>
<tr>
<th>U.S. Federal regulations</th>
<th>United States Inventory (TSCA 8b): This material is listed or exempted.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SARA 302/304/311/312 extremely hazardous substances: No products were found.</td>
</tr>
<tr>
<td></td>
<td>SARA 302/304 emergency planning and notification: No products were found.</td>
</tr>
<tr>
<td></td>
<td>SARA 302/304/311/312 hazardous chemicals: Carbon dioxide</td>
</tr>
<tr>
<td></td>
<td>SARA 311/312 MSDS distribution - chemical inventory - hazard identification:</td>
</tr>
<tr>
<td></td>
<td>Carbon dioxide: Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard</td>
</tr>
</tbody>
</table>

#### State regulations

| Connecticut Carcinogen Reporting: This material is not listed. |
| Connecticut Hazardous Material Survey: This material is not listed. |
| Florida substances: This material is not listed. |
| Illinois Chemical Safety Act: This material is not listed. |
| Illinois Toxic Substances Disclosure to Employee Act: This material is not listed. |
| Louisiana Reporting: This material is not listed. |
| Louisiana Spill: This material is not listed. |
| Massachusetts Spill: This material is not listed. |
| Massachusetts Substances: This material is listed. |
| Michigan Critical Material: This material is not listed. |
| Minnesota Hazardous Substances: This material is not listed. |
| New Jersey Hazardous Substances: This material is listed. |
| New Jersey Spill: This material is not listed. |
| New Jersey Toxic Catastrophe Prevention Act: This material is not listed. |
| New York Acutely Hazardous Substances: This material is not listed. |
| New York Toxic Chemical Release Reporting: This material is not listed. |
| Pennsylvania RTK Hazardous Substances: This material is listed. |
| Rhode Island Hazardous Substances: This material is not listed. |

#### Canada

<table>
<thead>
<tr>
<th>WHMIS (Canada)</th>
<th>Class A: Compressed gas.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CEPA Toxic substances: This material is listed.</td>
<td></td>
</tr>
<tr>
<td>Canadian ARET: This material is not listed.</td>
<td></td>
</tr>
<tr>
<td>Canadian NPR: This material is not listed.</td>
<td></td>
</tr>
<tr>
<td>Alberta Designated Substances: This material is not listed.</td>
<td></td>
</tr>
<tr>
<td>Ontario Designated Substances: This material is not listed.</td>
<td></td>
</tr>
<tr>
<td>Quebec Designated Substances: This material is not listed.</td>
<td></td>
</tr>
</tbody>
</table>

### Section 16. Other information

#### United States

<table>
<thead>
<tr>
<th>Label requirements</th>
<th>GAS:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CONTENTS UNDER PRESSURE.</td>
</tr>
<tr>
<td></td>
<td>MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.</td>
</tr>
<tr>
<td></td>
<td>CAN CAUSE TARGET ORGAN DAMAGE.</td>
</tr>
<tr>
<td></td>
<td>Do not puncture or incinerate container.</td>
</tr>
<tr>
<td></td>
<td>Can cause rapid suffocation.</td>
</tr>
<tr>
<td>LIQUID:</td>
<td>MAY CAUSE RESPIRATORY TRACT, EYE, AND SKIN IRRITATION.</td>
</tr>
<tr>
<td></td>
<td>CAN CAUSE TARGET ORGAN DAMAGE.</td>
</tr>
<tr>
<td></td>
<td>Extremely cold liquid and gas under pressure.</td>
</tr>
<tr>
<td></td>
<td>Can cause rapid suffocation.</td>
</tr>
<tr>
<td></td>
<td>May cause severe frostbite.</td>
</tr>
</tbody>
</table>

#### Canada

<table>
<thead>
<tr>
<th>Label requirements</th>
<th>Class A: Compressed gas.</th>
</tr>
</thead>
</table>
**Carbon Dioxide**

### Hazardous Material Information System (U.S.A.)

<table>
<thead>
<tr>
<th>Category</th>
<th>Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>1</td>
</tr>
<tr>
<td>Flammability</td>
<td>0</td>
</tr>
<tr>
<td>Physical hazards</td>
<td>0</td>
</tr>
</tbody>
</table>

### Liquid:

<table>
<thead>
<tr>
<th>Category</th>
<th>Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>Health</td>
<td>3</td>
</tr>
<tr>
<td>Fire hazard</td>
<td>0</td>
</tr>
<tr>
<td>Reactivity</td>
<td>0</td>
</tr>
<tr>
<td>Personal protection</td>
<td>0</td>
</tr>
</tbody>
</table>

### National Fire Protection Association (U.S.A.)

- **Flammability**
  - Health: 0
  - Instability: Special
- **Special**

---

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
Carbon Monoxide

Section 1. Chemical product and company identification

Product name: Carbon Monoxide
Supplier: AIRGAS INC., on behalf of its subsidiaries
258 North Rednor-Chester Road
Suite 100
Rednor, PA 19078-5283
1-610-987-5253

Product use: Synthetic/Analytical chemistry.
Synonym: Carbon oxide (CO); CO; Exhaust Gas; Flue gas; Carbonic oxide; Carbon oxide;
Carbon; Carbonio; Kohlenmonoxid; Kohlenoxyd; Koelmoxoxide; NA 9202; Oxyde de
carbon; UN 1016; Weglia tene: Flue gasnice; Carbon monoxide

MSDS #: 001014
Date of Preparation/Revision: 9/2/2010.
In case of emergency: 1-866-734-3438

Section 2. Hazards identification

Physical state: Gas. [COLORLESS GAS, MAY BE A LIQUID AT LOW TEMPERATURE OR HIGH
PRESSURE.]

Emergency overview: WARNING!
FLAMMABLE GAS.
MAY CAUSE FLASH FIRE.
MAY BE FATAL IF INHALED.
MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
CONTENTS UNDER PRESSURE.
Keep away from heat, sparks and flame. Do not puncture or incinerate container. Avoid
breathing gas. May cause target organ damage, based on animal data. Use only with
adequate ventilation. Keep container closed.
Contact with rapidly expanding gases can cause frostbite.

Target organs: May cause damage to the following organs: blood, lungs, cardiovascular system, central
nervous system (CNS).

Routes of entry: Inhalation
Potential acute health effects:
Eyes: Contact with rapidly expanding gas may cause burns or frostbite.
Skin: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation: Toxic by inhalation.
Ingestion: Ingestion is not a normal route of exposure for gases
Potential chronic health effects:
CARCINOGENIC EFFECTS: Not available.
MUTAGENIC EFFECTS: Not available.
TERATOGENIC EFFECTS: Classified 1 by European Union.

Medical conditions aggravated by over-exposure:
Pre-existing disorders involving any target organs mentioned in this MSDS as being at
risk may be aggravated by over-exposure to this product.

See toxicological information (section 11)
Section 3. Composition, Information on Ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS number</th>
<th>% Volume</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon Monoxide</td>
<td>630-08-0</td>
<td>100</td>
<td>ACGIH TLV (United States, 2/2010).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 29 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 25 ppm 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>NIOSH REL (United States, 6/2009).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CEIL: 229 mg/m³</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CEIL: 200 ppm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 40 mg/m³ 10 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 35 ppm 10 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>OSHA REL (United States, 11/2006).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 55 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 50 ppm 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CEIL: 229 mg/m³</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>CEIL: 200 ppm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 40 mg/m³ 8 hour(s).</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>TWA: 35 ppm 8 hour(s).</td>
</tr>
</tbody>
</table>

Section 4. First aid measures

No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

**Eye contact**
- Check for and remove any contact lenses. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical attention immediately.

**Skin contact**
- In case of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Wash clothing before reuse. Clean shoes thoroughly before reuse. Get medical attention immediately.

**Frothing**
- Try to warm up the frozen tissues and seek medical attention.

**Inhalation**
- Move exposed person to fresh air. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention immediately.

**Ingestion**
- As this product is a gas, refer to the ingestion section.

Section 5. Fire-fighting measures

- **Flammability of the product:** Flammable.
- **Auto-ignition temperature:** 608.89°C (1128°F)
- **Flammable limits:** Lower: 12.5% Upper: 74%
- **Products of combustion:** Decomposition products may include the following materials: carbon dioxide, carbon monoxide.
- **Fire hazards in the presence of various substances:** Extremely flammable in the presence of the following materials or conditions: open flames, sparks and static discharge and oxidizing materials.
- **Fire-fighting media and instructions:** In case of fire, use water spray (fog), foam or dry chemical.

In case of fire, allow gas to burn if flow cannot be shut off immediately. Apply water from a safe distance to cool container and protect surrounding area. If involved in fire, shut off flow immediately if it can be done without risk. Contains gas under pressure. Flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
Section 6. Accidental release measures

Personal precautions: Immediately contact emergency personnel. Keep unnecessary personnel away. Use suitable protective equipment (section 8). Shut off gas supply if this can be done safely. Isolate area until gas has dispersed.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up: Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see section 1 for emergency contact information and section 13 for waste disposal.

Section 7. Handling and storage

Handling: Use only with adequate ventilation. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. High pressure gas. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Keep container closed. Keep away from heat, sparks and flame. To avoid fire, eliminate ignition sources. Protect cylinders from physical damage; do not drop, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Storage: Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame). Segregate from oxidizing materials. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Engineering controls: Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

Eyes: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists or dusts.

Skin: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

The applicable standards are (US) 29 CFR 1910.134 and (Canada) 294.4.93

Hands: Chemical-resistant, impermeable gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Personal protection in case of a large spill: Self-contained breathing apparatus (SCBA) should be used to avoid inhalation of the product. Full chemical-resistant suit and self-contained breathing apparatus should be worn only by trained and authorized persons.

Product name: Carbon monoxide

ACGIH TLV (United States, 2/2010).
- TWA: 29 mg/m³ 8 hour(s).
- TWA: 25 ppm 8 hour(s).

NIOSH REL (United States, 6/2009).
- CEIL: 229 mg/m³
- CEIL: 200 ppm
- TWA: 40 mg/m³ 10 hour(s).
- TWA: 35 ppm 10 hour(s).

OSHA PEL (United States, 11/2006).
- TWA: 55 mg/m³ 8 hour(s).
**Carbon Monoxide**

TWA: 50 ppm 8 hour(s).
CEIL: 229 mg/m³
CEIL: 200 ppm
TWA: 40 mg/m³ 8 hour(s).
TWA: 35 ppm 8 hour(s).

Consult local authorities for acceptable exposure limits.

### Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>28.01 g/mole</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>C-O</td>
</tr>
<tr>
<td>Boiling/condensation point</td>
<td>-181.7°C (-313.1°F)</td>
</tr>
<tr>
<td>Melting/freezing point</td>
<td>-188.9°C (-336.1°F)</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>-140.1°C (-220.2°F)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>0.97 (Air = 1)</td>
</tr>
<tr>
<td>Specific Volume (ft³/lb)</td>
<td>13.8889</td>
</tr>
<tr>
<td>Gas Density (lb/ft³)</td>
<td>0.072</td>
</tr>
</tbody>
</table>

### Section 10. Stability and reactivity

- **Stability and reactivity**: The product is stable.
- **Incompatibility with various substances**: Extremely reactive or incompatible with the following materials: oxidizing materials.
- **Hazardous decomposition products**: Under normal conditions of storage and use, hazardous decomposition products should not be produced.
- **Hazardous polymerization**: Under normal conditions of storage and use, hazardous polymerization will not occur.

### Section 11. Toxicological information

#### Toxicity data

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>Result</th>
<th>Species</th>
<th>Dose</th>
<th>Exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon monoxide</td>
<td>TDL0 Intraperitoneal</td>
<td>Rat</td>
<td>35 mL/kg</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Vapor</td>
<td>Rat</td>
<td>15000 mg/m³</td>
<td>15 minutes</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Vapor</td>
<td>Rat</td>
<td>19000 mg/m³</td>
<td>4 hours</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Gas</td>
<td>Rat</td>
<td>3760 ppm</td>
<td>1 hours</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Gas</td>
<td>Mouse</td>
<td>2444 ppm</td>
<td>4 hours</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Gas</td>
<td>Rat</td>
<td>6600 ppm</td>
<td>30 minutes</td>
</tr>
<tr>
<td></td>
<td>LC50 Inhalation Gas</td>
<td>Rat</td>
<td>1807 ppm</td>
<td>4 hours</td>
</tr>
</tbody>
</table>

- **IDLH**: 1200 ppm

- **Chronic effects on humans**: TERATOGENIC EFFECTS: Classified 1 by European Union. May cause damage to the following organs: blood, lungs, cardiovascular system, central nervous system (CNS).

- **Other toxic effects on humans**: No specific information is available in our database regarding the other toxic effects of this material to humans.

- **Specific effects**
  - Carcinogenic effects: No known significant effects or critical hazards.
  - Mutagenic effects: No known significant effects or critical hazards.
  - Reproduction toxicity: No known significant effects or critical hazards.
Section 12. Ecological information

Aquatic ecotoxicity
Not available.

Products of degradation: Products of degradation: carbon oxides (CO, CO₂).
Environmental fate: Not available.
Environmental hazards: No known significant effects or critical hazards.
Toxicity to the environment: Not available.

Section 13. Disposal considerations

Product removed from the cylinder must be disposed of in accordance with appropriate Federal, State, local regulation. Return cylinders with residual product to Airgas, Inc. Do not dispose of locally.

Section 14. Transport information

<table>
<thead>
<tr>
<th>Regulatory Information</th>
<th>UN number</th>
<th>Proper shipping name</th>
<th>Class</th>
<th>Packing group</th>
<th>Label</th>
<th>Additional Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOT Classification</td>
<td>UN1016</td>
<td>CARBON MONOXIDE, COMPRESSED</td>
<td>2.3</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Limited quantity Yes. Packaging instruction Passenger aircraft Quantity limitation: Forbidden. Cargo aircraft Quantity limitation: 25 kg Special provisions 4</td>
</tr>
<tr>
<td>TDG Classification</td>
<td>UN1016</td>
<td>CARBON MONOXIDE, COMPRESSED</td>
<td>2.3</td>
<td>Not applicable (gas).</td>
<td></td>
<td>Explosive Limit and Limited Quantity Index 0 FRAP Index 0 Passenger Carrying Ship Index Forbidden Passenger Carrying Road or Rail Index Forbidden</td>
</tr>
</tbody>
</table>

Page: 5/7
### Section 15. Regulatory information

**United States**
- **U.S. Federal regulations**: United States inventory (TSCA 8b): This material is listed or exempted.
  - SARA 302/304/311/312 extremely hazardous substances: No products were found.
  - SARA 302/304 emergency planning and notification: No products were found.
  - SARA 302/304/311/312 hazardous chemicals: Carbon monoxide
  - SARA 311/312 MSDS distribution - chemical inventory - hazard identification:
    - Carbon monoxide: Fire hazard, Sudden release of pressure, Immediate (acute) health hazard, Delayed (chronic) health hazard
  - Clean Water Act (CWA) 307: No products were found.
  - Clean Water Act (CWA) 311: No products were found.
  - Clean Air Act (CAA) 112 accidental release prevention: No products were found.
  - Clean Air Act (CAA) 112 regulated flammable substances: No products were found.
  - Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

**State regulations**: Connecticut Carcinogen Reporting: This material is not listed.
- Connecticut Hazardous Material Survey: This material is not listed.
- Florida substances: This material is not listed.
- Illinois Chemical Safety Act: This material is not listed.
- Illinois Toxic Substances Disclosure to Employee Act: This material is not listed.
- Louisiana Reporting: This material is not listed.
- Louisiana Spill: This material is not listed.
- Massachusetts Spill: This material is not listed.
- Massachusetts Substances: This material is listed.
- Michigan Critical Material: This material is not listed.
- Minnesota Hazardous Substances: This material is not listed.
- New Jersey Hazardous Substances: This material is listed.
- New Jersey Spill: This material is not listed.
- New Jersey Toxic Catastrophe Prevention Act: This material is listed.
- New York Acutely Hazardous Substances: This material is not listed.
- New York Toxic Chemical Release Reporting: This material is listed.
- Pennsylvania RTK Hazardous Substances: This material is listed.
- Rhode Island Hazardous Substances: This material is not listed.

**California Prop. 65**: WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

**Ingredient name**
- **Cancer**: No.
- **Reproductive**: Yes.
- **No significant risk level**: No.
- **Maximum acceptable dosage level**: No.

**Canada**
- **WHMIS (Canada)**: Class A: Compressed gas.
  - Class B-1: Flammable gas.
  - Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
  - Class D-2A: Material causing other toxic effects (Very toxic).
### Section XII: Appendices

#### Carbon Monoxide

- **CEPA Toxic substances**: This material is not listed.
- **Canadian ARET**: This material is not listed.
- **Canadian NPRI**: This material is listed.
- **Alberta Designated Substances**: This material is not listed.
- **Ontario Designated Substances**: This material is not listed.
- **Quebec Designated Substances**: This material is not listed.

### Section 16. Other information

**United States**

**Label requirements**
- FLAMMABLE GAS.
- MAY CAUSE FLASH FIRE.
- MAY BE FATAL IF INHALED.
- MAY CAUSE TARGET ORGAN DAMAGE, BASED ON ANIMAL DATA.
- CONTENTS UNDER PRESSURE.

**Canada**

**Label requirements**
- Class A: Compressed gas.
- Class B-1: Flammable gas.
- Class D-1A: Material causing immediate and serious toxic effects (Very toxic).
- Class D-2A: Material causing other toxic effects (Very toxic).

**Hazardous Material Information System (U.S.A.)**

<table>
<thead>
<tr>
<th>Health</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flammability</td>
</tr>
<tr>
<td>Physical hazards</td>
</tr>
</tbody>
</table>

**National Fire Protection Association (U.S.A.)**

<table>
<thead>
<tr>
<th>Health</th>
<th>Flammability</th>
<th>Instability</th>
<th>Special</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notice to reader**

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
Material Safety Data Sheet
Sodium nitrate MSDS

Section 1: Chemical Product and Company Identification
Product Name: Sodium nitrate
Catalog Codes: SLS1102, SLS3946, SLS1726
CAS#: 7631-09-4
RTECS: WC5600000
TSCA: TSCA (b) Inventory: Sodium nitrate
Cl#: Not available.
Synonym: Chile saltpeter; soda niter; Sodium salt peter; Nitric acid; sodium salt; Nitrates
Chemical Name: Sodium Nitrate
Chemical Formula: NaNO3
Contact Information:
ScienceLab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396
US Sales: 1-800-601-7247
International Sales: 1-281-441-4400
Order Online: ScienceLab.com
CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300
International CHEMTREC, call: 1-703-527-3887
For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients
Composition:

<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>% by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sodium nitrate</td>
<td>7631-09-4</td>
<td>100</td>
</tr>
</tbody>
</table>

Toxicological Data on Ingredients: Sodium nitrate: ORAL (LD50): Acute: 1267 mg/kg [Rat]. 2590 mg/kg [Rabbit].

Section 3: Hazards Identification
Potential Acute Health Effects:
Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant). On eye contact (irritant), of inhalation. Prolonged exposure may result in skin burns and ulcers. Over-exposure by inhalation may cause respiratory irritation.
Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures
Eye Contact:
Section XII: Appendices

Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention if irritation occurs.

**Skin Contact:**
Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

**Serious Skin Contact:** Not available.

**Inhalation:**
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

**Serious Inhalation:**
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

**Ingestion:**
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or wristband.

**Serious Ingestion:** Not available.

---

**Section 5: Fire and Explosion Data**

**Flammability of the Product:** Non-flammable.

**Auto-Ignition Temperature:** Not applicable.

**Flash Points:** Not applicable.

**Flammable Limits:** Not applicable.

**Products of Combustion:** Not available.

**Fire Hazards in Presence of Various Substances:** organic materials, combustible materials

**Explosion Hazards in Presence of Various Substances:**

**Fire Fighting Media and Instructions:** Not applicable.

**Special Remarks on Fire Hazards:**
It may accelerate burning when involved in a fire. Increases the flammability of any combustible material. May ignite combustibles (wood, paper, clothing, etc.). Flames up when heated to 540 deg. C. Mixture with charcoal ignites on heating. Contact with combustible or organic materials may cause fire.

**Special Remarks on Explosion Hazards:**
It will react explosively with hydrocarbons. Interaction of nitrates when heated with amidosulfates/sulfamates may become explosively violent owing to liberation of dinitrogen oxide and steam. Mixtures of sodium nitrate with powdered aluminum or its oxide were reported to be explosive. Mixtures of sodium nitrate and barium thiocyanate may explode. Mixture with sodium nitrate and powdered antimony explode. Mixture of sodium nitrate and sodium thiosulfate or sodium phosphinate explode.

---

**Section 6: Accidental Release Measures**

**Small Spill:** Use appropriate tools to put the spilled solid in a convenient waste disposal container.

**Large Spill:**
Oxidizing material. Stop leak if without risk. Avoid contact with a combustible material (wood, paper, oil, clothing, etc.). Keep substance damp using water spray. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Call for assistance on disposal.
Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Keep away from combustible material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label. Keep away from incompatibles such as reducing agents, combustible materials, organic materials, acids.

Storage:

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Safety glasses. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient. Consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Granular solid. Powdered solid.)
Odor: Not available.
Molecular Weight: 84.99 g/mole
Color: White.

pH (1% soln/water): Not available.
Boiling Point: Decomposition temperature: 380°C (716°F)
Melting Point: 303°C (586.4°F)

Critical Temperature: Not available.
Specific Gravity: Density: 2.25 (Water = 1)
Vapor Pressure: Not applicable.
Vapor Density: Not available.
Volatile: Not available.
Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.
Ionicity (in Water): Not available.
Dispersion Properties: See solubility in water, methanol.
Solubility:
Easily soluble in hot water. Soluble in cold water. Partially soluble in methanol. Very slightly soluble in acetone. Very slightly soluble in glycerol. Very soluble in liquid Ammonia. Solubility in water: 92.1 g/100 ml @ 25 deg. C., 190 g/100 ml @ 100 deg. C. Solubility in Methanol: 1 g dissolves in 300 ml Methanol 1 gram dissolves in 125 ml Alcohol, 52 ml boiling Alcohol, 3470 ml absolute Alcohol.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Incompatible materials.
Incompatibility with various substances: Highly reactive with combustible materials, organic materials. Reactive with reducing agents, acids.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity: Fibrous organic material is oxidized in contact with sodium nitrate above 100 deg. C. and will ignite below 220 C. Wood and similar cellulose materials are rendered highly combustible by nitrate impregnation. Reacts with acids to emit toxic fumes of nitrogen dioxide. Also incompatible with boron phosphide, barium rhodanide, cyanides, sodium thiosulfate, hypophosphites such as sodium hypophosphate, sulfur plus charcoal, antimony, chlorides, aluminum and stannous chloride, esters, powdered metals such as zinc or aluminum or aluminum oxide, isothiocyanates, thiocyanates, phosphorus, organic materials, combustible materials, acids, pyrosulfites, sulfides, amides, bisulfites, hydrozinc, ammonium sulfate, amides, amines, phospham. Sodium nitrate + amines may for nitroamines which have been proven to be carcinogenic in animal tests.
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation, Ingestion.
Toxicity to Animals: Acute oral toxicity (LD50): 1267 mg/kg [Rat].

Chronic Effects on Humans:
MUTAGENIC EFFECTS: Mutagenic for bacteria and/or yeast. May cause damage to the following organs: blood.

Other Toxic Effects on Humans:
Hazardous in case of ingestion. Slightly hazardous in case of skin contact (irritant), of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May affect genetic material (mutagenic). May cause adverse reproductive effects based on animal test data. May cause cancer based on animal test data.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation with redness, itching, and pain. Eyes: Causes eye irritation with redness, itching, and pain. Inhalation: Causes respiratory tract and mucous membrane irritation. Symptoms may include coughing, shortness of breath. Ingestion: May be harmful if swallowed. Clinical signs associated with nitrate poisoning include: Gastroenteritis, abdominal pain, nausea, vomiting, diarrhea, metabolis acidosis, muscular weakness, dizziness, fatigue, headache, mental impairment, incoordination, convulsions, accelerated heart rate, orthostatic hypotension, dyspnea, and in severe cases, methemoglobinemia due to inadequate oxygenation of the blood leading to progressive cyanosis, and coma. Cyanosis is first visible as a bluish discolouration of the mucous membranes and unpigmented areas of the body. Purging and diuresis can be expected. Rare cases of nitrates being converted into more toxic nitrates.

Section 12: Ecological Information
Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 5.1: Oxidizing material.
Identification: Sodium nitrate UNNA: 1498 PG: III
Special Provisions for Transport: Non- Pollutant

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey: Sodium nitrate Rhode Island RTK hazardous substances: Sodium nitrate Pennsylvania RTK: Sodium nitrate Massachusetts RTK: Sodium nitrate New Jersey: Sodium nitrate TSCA 8(b) inventory: Sodium nitrate

Other Regulations:

Other Classifications:
WHMIS (Canada):
CLASS C: Oxidizing Material CLASS D-2B: Material causing other toxic effects (TOXIC).

DSCL (EEC):
R8- Contact with combustible material may cause fire. R22- Harmful if swallowed. S17- Keep away from combustible material. S36- Wear suitable protective clothing.

HMIS (U.S.A.):
Health Hazard: 2
Fire Hazard: 0
Reactivity: 0
Personal Protection: E

National Fire Protection Association (U.S.A.):
Health: 2
Flammability: 0
Reactivity: 0
### Section XII: Appendices

**Specific hazard:**

**Protective Equipment:**
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Safety glasses.

### Section 16: Other Information

**References:** Not available.

**Other Special Considerations:** Not available.

**Created:** 10/10/2005 08:27 PM

**Last Updated:** 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.
Material Safety Data Sheet
Potassium nitrate MSDS

Section 1: Chemical Product and Company Identification

| Product Name: Potassium nitrate                  | Contact Information:               |
| Catalog Codes: SLP4009, SLP3001, SLP4815, SLP1987 | Sciencelab.com, Inc.               |
| CAS#: 7757-79-1                                   | 14025 Smith Rd.                    |
| RTECS: TT370000                                   | Houston, Texas 77396               |
| TSCA: TSCA 8(b) inventory: Potassium nitrate      | US Sales: 1-800-901-7247           |
| Cl#: Not available                                | International Sales: 1-281-441-4400|
| Synonym: Nitric Acid, potassium salt, saltpeter   | Order Online: Sciencelab.com       |
| Chemical Name: Potassium Nitrate                  | CHEMTREC (24HR Emergency Telephone), call: |
| Chemical Formula: KNO₃                             | 1-800-424-9300                      |
|                                                   | International CHEMTREC, call: 1-703-527-3887|
|                                                   | For non-emergency assistance, call: 1-281-441-4400|

Section 2: Composition and Information on Ingredients

| Composition: |
| Name | CAS # | % by Weight |
| Potassium nitrate | 7757-79-1 | 100 |

Toxicological Data on Ingredients: Potassium nitrate: ORAL (LD50): Acute: 3750 mg/kg [Rat], 1901 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation (lung irritant). Prolonged exposure may result in skin bums and ulcerations. Over-exposure by inhalation may cause respiratory irritation.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance may be toxic to blood, kidneys, central nervous system (CNS). Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.
Section XII: Appendices

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Cold water may be used. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 6: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of static discharge: Not available. Slightly explosive in presence of shocks, of heat.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards:
In contact with easily oxidizable substances, it may react rapidly enough to cause ignition, violent combustion, or explosion. It increases the flammability of any combustible substance. A mixture of potassium nitrate and calcium silicide is a readily ignited primer and burns at a very high temperature. Contact of the carbide with molten potassium nitrate causes incandescence. When heated to decomposition it emits very toxic fumes.

Special Remarks on Explosion Hazards:
A mixture of potassium nitrate and antimony trisulfide explodes when heated. When copper phosphide is mixed with potassium nitrate and heated, it explodes. Mixture of germanium nitrate and potassium nitrate explodes when heated. A mixture of potassium nitrate, sulfur, arsenic trisulfide is known as a pyrotechnic formulation. When titanium is heated with potassium nitrate, an explosion occurs. A mixture of potassium nitrate and titanium disulfide explodes when heated. When potassium nitrate is mixed with boron, tin, and trichloroethylene an explosion can occur. Powdered zinc and potassium explode if heated. Arsenic disulfide forms explosive mixtures when mixed with potassium nitrate. Charcoal (powdered carbon) and potassium nitrate make a pyrotechnic mixture. Contact at 290 °C causes a vigorous combustion and the mixture explodes on heating. A mixture of potassium nitrate and sodium acetate may cause an explosion. A mixture of potassium nitrate and sodium hydrosulfite constitutes a powerful explosive. Mixtures of potassium nitrate with sodium phosphinate and sodium thiocyanate are explosive.
Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Oxidizing material. Stop leak if without risk. Avoid contact with a combustible material (wood, paper, oil, clothing...). Keep substance damp using water spray. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; diko if needed. Call for assistance on disposal.

Section 7: Handling and Storage

Precautions:
Keep away from heat. Keep away from sources of ignition. Keep away from combustible material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as reducing agents, combustible materials, organic materials, metals.

Storage:

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Crystalline solid. Granular solid.)
Odor: Odorless.
Taste: Cooling, Saline. Pungent.
Molecular Weight: 101.1 g/mole
Color: White.

pH (1% soln/water): Not available.

Boiling Point: Decomposition temperature: 400°C (752°F)

Melting Point: 334°C (633.2°F)

Critical Temperature: Not available.

Specific Gravity: 2.109 (Water = 1) @ 16 degrees C
Section XII: Appendices

Vapor Pressure: Not applicable.
Vapor Density: Not available.
Volatile: Not available.
Odor Threshold: Not available.
Water/Oil Dist. Coeff.: Not available.
Ionicity (in Water): Not available.
Dispersion Properties: See solubility in water.
Solubility:
Easily soluble in hot water. Soluble in cold water. Insoluble in diethyl ether. Soluble in liquid ammonia, glycerin, and absolute alcohol. Solubility in water: 1g/2.8 ml water @ 25 °C; 13.3 g/100 ml water @ 0 °C; 1g/0.5 ml boiling water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.
Conditions of Instability: Incompatible materials, dust generation
Incompatibility with various substances: Reactive with reducing agents, combustible materials, organic materials, metals.
Corrosivity: Non-corrosive in presence of glass.
Special Remarks on Reactivity:
Hygroscopic; keep container tightly closed. Potassium nitrate reacts vigorously when heated with sulfides of the alkaline earth group including barium sulfide and calcium sulfide. Also incompatible with boron, and finely powdered metals, chromium nitride, aluminum, titanium, antimony, germanium, zinc, zirconium, calcium disilicide, metal sulfides, carbon, sulfur, phosphorus, phosphides, sodium phosphate, sodium thiosulfate, citric acid, tin chloride, sodium acetate, threon carbide.
Special Remarks on Corrosivity: Not available.
Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.
Toxicity to Animals: Acute oral toxicity (LD50): 1901 mg/kg [Rabbit].
Chronic Effects on Humans: May cause damage to the following organs: blood, kidneys, central nervous system (CNS).
Other Toxic Effects on Humans: Hazardous in case of skin contact (irritant), of ingestion, of inhalation (lung irritant).
Special Remarks on Toxicity to Animals: Not available.
Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects based on animal test data. May affect genetic material (mutagenic)
Special Remarks on other Toxic Effects on Humans:
Acute Potent Health Effects: Skin: Causes skin irritation. Eyes: Causes eye irritation Inhalation: Breathing Potassium Nitrate can irritate the nose and throat causing sneezing and coughing. High levels can interfere with the ability of the blood to carry oxygen causing headache, dizziness and a blue color to the skin and lips (methemoglobinemia), and other symptoms of methemoglobinemia (see other symptoms under ingestion). Higher levels can cause trouble breathing, circulatory collapse and even death. Ingestion: Ingestion of large quantities may cause violent gastroenteritis with nausea, vomiting, severe abdominal pain. It may also cause colic and diarrhea. Acute toxicity of nitrate occurs as a result of reduction to nitrite. The nitrite acts in the blood to oxidize hemoglobin to methemoglobin which does not perform as an oxygen carrier to tissues causing Methemoglobinemia. Symptoms may include vertigo, muscular weakness, syncope, irregular pulse, convulsions.
anoxia, coma, fall in blood pressure, roaring sound in the ears, a persistent throbbing headache, generalized tingling sensation, heart palpitations, visual disturbances caused by increased intracocular tension and intracranial pressure, flushed and perspiring skin, which is later cold and cyanotic. Circulatory collapse and death may occur. Chronic Potential Health Effects: Ingestion and Inhalation: Repeated or prolonged exposure to small amounts may affect the blood, respiration and kidneys and produce anemia. Methemoglobinemia with attendant cyanosis and anoxia, hyperpnea and later dyspnea, and nephritis.

Section 12: Ecological Information

Ecotoxicity: Not available.
BOD5 and COD: Not available.
Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.
Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 5.1: Oxidizing material.
Identification: Potassium nitrate: UN1486 PG. III
Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Connecticut hazardous material survey: Potassium nitrate Rhode Island RTK hazardous substances: Potassium nitrate Pennsylvania RTK: Potassium nitrate Massachusetts RTK: Potassium nitrate TSCA 8(b) inventory: Potassium nitrate
Other Regulations:
Other Classifications:
WHMIS (Canada): CLASS C: Oxidizing material.
DSCL (EEC):
HMIS (U.S.A.):
    Health Hazard: 2
    Fire Hazard: 0
    Reactivity: 0
    Personal Protection: E
National Fire Protection Association (U.S.A.):
### Health: 2

- Flammability: 0
- Reactivity: 0

### Protective Equipment:
- Gloves, Lab coat, Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

## Section 16: Other Information

**References:** Not available.

**Other Special Considerations:** Not available.

**Created:** 10/10/2005 08:23 PM

**Last Updated:** 11/01/2010 12:00 PM

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall ScienceLab.com be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, however arising, even if ScienceLab.com has been advised of the possibility of such damages.

---

Appendix E: Sample ASPEN Block Reports
BLOCK: CMP-300 MODEL: MCOMPR

INLET STREAMS: S-325 TO STAGE 1
OUTLET STREAMS: S-314 FROM STAGE 4
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE (LBMOL/HR)</td>
<td>3681.00</td>
<td>3681.00</td>
<td>0.00000</td>
</tr>
<tr>
<td>MASS (LB/HR)</td>
<td>7420.46</td>
<td>7420.46</td>
<td>0.00000</td>
</tr>
<tr>
<td>ENTHALPY (BTU/HR)</td>
<td>0.160078E+07</td>
<td>0.278814E+08</td>
<td>-0.942586</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION 0.00000 LB/HR

*** INPUT DATA ***

ISENTROPIC CENTRIFUGAL COMPRESSOR
NUMBER OF STAGES 4
FINAL PRESSURE, PSIA 1,166.30

COMPRESSOR SPECIFICATIONS PER STAGE

<table>
<thead>
<tr>
<th>STAGE NUMBER</th>
<th>MECHANICAL EFFICIENCY</th>
<th>ISENTROPIC EFFICIENCY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.000</td>
<td>0.7200</td>
</tr>
<tr>
<td>2</td>
<td>1.000</td>
<td>0.7200</td>
</tr>
<tr>
<td>3</td>
<td>1.000</td>
<td>0.7200</td>
</tr>
<tr>
<td>4</td>
<td>1.000</td>
<td>0.7200</td>
</tr>
</tbody>
</table>

COOLER SPECIFICATIONS PER STAGE

<table>
<thead>
<tr>
<th>STAGE NUMBER</th>
<th>PRESSURE DROP</th>
<th>TEMPERATURE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PSI</td>
<td>F</td>
</tr>
</tbody>
</table>
### Section XII: Appendices

#### *** RESULTS ***

<table>
<thead>
<tr>
<th>STAGE</th>
<th>OUTLET PRESSURE</th>
<th>OUTLET RATIO</th>
<th>TEMPERATURE°F</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>43.86</td>
<td>2.985</td>
<td>444.3</td>
</tr>
<tr>
<td>2</td>
<td>130.9</td>
<td>3.127</td>
<td>996.9</td>
</tr>
<tr>
<td>3</td>
<td>390.8</td>
<td>3.031</td>
<td>1387.</td>
</tr>
<tr>
<td>4</td>
<td>1166.</td>
<td>3.000</td>
<td>1775.</td>
</tr>
</tbody>
</table>

#### *** PROFILE ***

### COMPRESSOR PROFILE

<table>
<thead>
<tr>
<th>STAGE</th>
<th>INDICATED HORSEPOWER</th>
<th>BRAKE HORSEPOWER</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3073.</td>
<td>3073.</td>
</tr>
<tr>
<td>2</td>
<td>5124.</td>
<td>5124.</td>
</tr>
<tr>
<td>3</td>
<td>6392.</td>
<td>6392.</td>
</tr>
<tr>
<td>4</td>
<td>7751.</td>
<td>7751.</td>
</tr>
</tbody>
</table>

### COOLER PROFILE

<table>
<thead>
<tr>
<th>STAGE</th>
<th>HEAD FLOW</th>
<th>VOLUMETRIC FLOW</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5905E+06</td>
<td>0.1613E+07</td>
</tr>
<tr>
<td>2</td>
<td>0.9844E+06</td>
<td>0.8998E+06</td>
</tr>
<tr>
<td>3</td>
<td>0.1228E+07</td>
<td>0.3767E+06</td>
</tr>
<tr>
<td>4</td>
<td>0.1489E+07</td>
<td>0.1533E+06</td>
</tr>
</tbody>
</table>
CASTILLO, ERNST, LERCH, WINCHESTER

STAGE           OUTLET          OUTLET          COOLING          VAPOR
NUMBER          TEMPERATURE     PRESSURE     LOAD        FRACTION
              F              PSIA         BTU/HR

1          493.0           41.86       0.1254E+07   1.000
2          767.0           128.9     -.5957E+07    1.000
3          1041.           388.8     -.9116E+07    1.000
4          1150.           1164.     -.1674E+08    1.000

BLOCK: DC-500  MODEL: RADFRAC

-------------------------------
INLETS - S-504 STAGE 12
OUTLETS - S-512 STAGE 1
S-505 STAGE 30
HS-706 STAGE 30
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN          OUT        RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR)       3769.17       3769.17         0.00000
MASS(LB/HR )         358212.       358212.        0.399806E-07
ENTHALPY(BTU/HR )   -0.502864E+08 -0.809244E+08    0.378600

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E             0.00000         LB/HR
PRODUCT STREAMS CO2E          0.00000         LB/HR
NET STREAMS CO2E PRODUCTION   0.00000         LB/HR
UTILITIES CO2E PRODUCTION     0.00000         LB/HR
TOTAL CO2E PRODUCTION         0.00000         LB/HR

**********************
**** INPUT DATA ****
**********************

**** INPUT PARAMETERS ****

NUMBER OF STAGES            30
ALGORITHM OPTION            STANDARD
ABSORBER OPTION            NO
INITIALIZATION OPTION: STANDARD
HYDRAULIC PARAMETER CALCULATIONS: NO
INSIDE LOOP CONVERGENCE METHOD: BROYDEN
DESIGN SPECIFICATION METHOD: NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS: 200
MAXIMUM NO. OF INSIDE LOOP ITERATIONS: 10
MAXIMUM NUMBER OF FLASH ITERATIONS: 30
FLASH TOLERANCE: 0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE: 0.000100000

**** COL-SPECS ****
MOLAR VAPOR DIST / TOTAL DIST: 1.00000
MASS REFLUX RATIO: 0.86000
MASS DISTILLATE TO FEED RATIO: 0.60000

**** PROFILES ****
P-SPEC STAGE 1 PRES, PSIA: 14.6959

**** TRAY MURPHREE EFFICIENCY ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>EFFICIENCY</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.56000</td>
</tr>
<tr>
<td>4</td>
<td>0.56000</td>
</tr>
<tr>
<td>5</td>
<td>0.56000</td>
</tr>
<tr>
<td>6</td>
<td>0.56000</td>
</tr>
<tr>
<td>7</td>
<td>0.56000</td>
</tr>
<tr>
<td>8</td>
<td>0.57000</td>
</tr>
<tr>
<td>9</td>
<td>0.57000</td>
</tr>
<tr>
<td>10</td>
<td>0.57000</td>
</tr>
<tr>
<td>11</td>
<td>0.57000</td>
</tr>
<tr>
<td>12</td>
<td>0.57000</td>
</tr>
<tr>
<td>13</td>
<td>0.58000</td>
</tr>
<tr>
<td>14</td>
<td>0.58000</td>
</tr>
<tr>
<td>15</td>
<td>0.59000</td>
</tr>
<tr>
<td>16</td>
<td>0.59000</td>
</tr>
<tr>
<td>17</td>
<td>0.59000</td>
</tr>
<tr>
<td>18</td>
<td>0.60000</td>
</tr>
<tr>
<td>19</td>
<td>0.60000</td>
</tr>
<tr>
<td>20</td>
<td>0.60000</td>
</tr>
<tr>
<td>21</td>
<td>0.60000</td>
</tr>
</tbody>
</table>
Castillo, Ernst, Lerch, Winchester

22  0.60000
23  0.60000
24  0.60000
25  0.60000
26  0.60000
27  0.60000
28  0.60000
29  0.60000

*********************
**** RESULTS ****
*********************

*** COMPONENT SPLIT FRACTIONS ***

OUTLET STREAMS
--------------
S-512    S-505

COMPONENT:
P-XYL   .79372E-01  .92063
O-XYL   .32804E-01  .96720
M-XYL   .70713E-01  .92929
N-BUTANE 1.0000   0.0000
N-PENT  1.0000   .36308E-14
N-HEX   1.0000   .70792E-09
WATER   1.0000   0.0000
H2      1.0000   0.0000
ETHYLBEN .11302  .88698
TOLUENE .95549  .44512E-01
BENZENE 1.0000   .70753E-06
NAPTH   .95419E-05 .99999
1:2:4-01  .60681E-03 .99939
ISOPR-01 .10042E-01  .98996
N-HEP-01 .99997  .31569E-04
1-BUT-01 1.0000   0.0000
1-PEN-01 1.0000   0.0000
1-HEX-01 1.0000   .16512E-09
1-HEP-01 .99999  .11951E-04

*** SUMMARY OF KEY RESULTS ***

468
### TOP STAGE TEMPERATURE
F  209.002

### BOTTOM STAGE TEMPERATURE
F  296.357

### TOP STAGE LIQUID FLOW
LBMOL/HR  2,021.01

### BOTTOM STAGE LIQUID FLOW
LBMOL/HR  1,271.21

### TOP STAGE VAPOR FLOW
LBMOL/HR  2,497.96

### BOILUP VAPOR FLOW
LBMOL/HR  4,599.15

### MOLAR REFLUX RATIO
0.80906

### MOLAR BOILUP RATIO
3.61793

### CONDENSER DUTY (W/O SUBCOOL)
BTU/HR  -0.306380+08

### REBOILER DUTY
BTU/HR  0.754021+08

** **** MAXIMUM FINAL RELATIVE ERRORS **** **

### DEW POINT
0.66479E-06 STAGE= 16

### BUBBLE POINT
0.35497E-06 STAGE= 17

### COMPONENT MASS BALANCE
0.72927E-06 STAGE= 30 COMP=NAPTH

### ENERGY BALANCE
0.13476E-06 STAGE= 2

** **** PROFILES **** **

**NOTE** REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

### ENTHALPY

<table>
<thead>
<tr>
<th>STAGE TEMPERATURE</th>
<th>PRESSURE</th>
<th>BTU/LBMOL</th>
<th>HEAT DUTY</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>PSIA</td>
<td>LIQUID</td>
<td>VAPOR</td>
</tr>
<tr>
<td>1</td>
<td>209.00</td>
<td>-429.49</td>
<td>-4577.9</td>
</tr>
<tr>
<td>2</td>
<td>221.14</td>
<td>3955.2</td>
<td>4057.3</td>
</tr>
<tr>
<td>10</td>
<td>231.40</td>
<td>3428.8</td>
<td>5935.7</td>
</tr>
<tr>
<td>11</td>
<td>232.48</td>
<td>3159.6</td>
<td>5820.2</td>
</tr>
<tr>
<td>12</td>
<td>229.92</td>
<td>1569.8</td>
<td>5709.9</td>
</tr>
<tr>
<td>13</td>
<td>242.19</td>
<td>5237.0</td>
<td>16521.</td>
</tr>
<tr>
<td>14</td>
<td>246.46</td>
<td>6640.6</td>
<td>20753.</td>
</tr>
<tr>
<td>15</td>
<td>248.25</td>
<td>7201.8</td>
<td>22398.</td>
</tr>
<tr>
<td>16</td>
<td>249.27</td>
<td>7402.3</td>
<td>23073.</td>
</tr>
<tr>
<td>17</td>
<td>250.10</td>
<td>7420.0</td>
<td>23327.</td>
</tr>
<tr>
<td>29</td>
<td>283.89</td>
<td>1337.3</td>
<td>16874.</td>
</tr>
<tr>
<td>30</td>
<td>296.36</td>
<td>4651.5</td>
<td>16816.</td>
</tr>
</tbody>
</table>

469
<table>
<thead>
<tr>
<th>STAGE</th>
<th>FLOW RATE</th>
<th>FEED RATE</th>
<th>PRODUCT RATE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LB/MOL/HR</td>
<td>LB/MOL/HR</td>
<td>LB/MOL/HR</td>
</tr>
<tr>
<td></td>
<td>LIQUID</td>
<td>VAPOR</td>
<td>LIQUID</td>
</tr>
<tr>
<td>1</td>
<td>2021.</td>
<td>2498.</td>
<td>2497.9640</td>
</tr>
<tr>
<td>2</td>
<td>2034.</td>
<td>4519.</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1950.</td>
<td>4461.</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>1975.</td>
<td>4448.</td>
<td>2.2144</td>
</tr>
<tr>
<td>12</td>
<td>6052.</td>
<td>4471.</td>
<td>3766.9596</td>
</tr>
<tr>
<td>13</td>
<td>6179.</td>
<td>4781.</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>6217.</td>
<td>4908.</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>6226.</td>
<td>4946.</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>6226.</td>
<td>4955.</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>6220.</td>
<td>4955.</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>5870.</td>
<td>4723.</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1271.</td>
<td>4599.</td>
<td>1271.2100</td>
</tr>
</tbody>
</table>

**** MASS FLOW PROFILES ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>FLOW RATE</th>
<th>FEED RATE</th>
<th>PRODUCT RATE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LB/HR</td>
<td>LB/HR</td>
<td>LB/HR</td>
</tr>
<tr>
<td></td>
<td>LIQUID</td>
<td>VAPOR</td>
<td>LIQUID</td>
</tr>
<tr>
<td>1</td>
<td>1.0184E+06</td>
<td>0.2149E+06</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1.0181E+06</td>
<td>0.3998E+06</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>1.0186E+06</td>
<td>0.4020E+06</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>1.0190E+06</td>
<td>0.4017E+06</td>
<td>145.4036</td>
</tr>
<tr>
<td>12</td>
<td>0.5916E+06</td>
<td>0.4050E+06</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.6082E+06</td>
<td>0.4484E+06</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0.6134E+06</td>
<td>0.4649E+06</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>0.6153E+06</td>
<td>0.4701E+06</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0.6162E+06</td>
<td>0.4720E+06</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.6169E+06</td>
<td>0.4729E+06</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>0.6410E+06</td>
<td>0.5031E+06</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.1433E+06</td>
<td>0.4977E+06</td>
<td>14328+06</td>
</tr>
</tbody>
</table>

**** MOLE-X-PROFILE ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>P-XYL</th>
<th>O-XYL</th>
<th>M-XYL</th>
<th>N-BUTANE</th>
<th>N-PENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3730E-01</td>
<td>0.10023E-02</td>
<td>0.32578E-02</td>
<td>0.17011E-02</td>
<td>0.19042E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.54109E-01</td>
<td>0.15527E-02</td>
<td>0.47695E-02</td>
<td>0.70336E-03</td>
<td>0.88759E-02</td>
</tr>
<tr>
<td>10</td>
<td>0.16600</td>
<td>0.76331E-02</td>
<td>0.15566E-01</td>
<td>0.60103E-03</td>
<td>0.68752E-02</td>
</tr>
<tr>
<td>11</td>
<td>0.17227</td>
<td>0.83923E-02</td>
<td>0.16265E-01</td>
<td>0.60093E-03</td>
<td>0.68530E-02</td>
</tr>
<tr>
<td>12</td>
<td>0.16731</td>
<td>0.91587E-02</td>
<td>0.16009E-01</td>
<td>0.10045E-02</td>
<td>0.10841E-01</td>
</tr>
<tr>
<td>Stage</td>
<td>Benzene</td>
<td>Napth</td>
<td>1:2:4-1</td>
<td>ISOPR-1</td>
<td>N-HEP-1</td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>-------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
</tr>
<tr>
<td>1</td>
<td>0.86395E-02</td>
<td>0.21431E-05</td>
<td>0.11894E-03</td>
<td>0.24509E-02</td>
<td>0.23302E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.60301E-02</td>
<td>0.52184E-05</td>
<td>0.23587E-03</td>
<td>0.41058E-02</td>
<td>0.18333E-01</td>
</tr>
<tr>
<td>10</td>
<td>0.49632E-02</td>
<td>0.27589E-01</td>
<td>0.33993E-01</td>
<td>0.60303E-01</td>
<td>0.13546E-01</td>
</tr>
<tr>
<td>11</td>
<td>0.30682E-02</td>
<td>0.27143E-01</td>
<td>0.33834E-01</td>
<td>0.60813E-01</td>
<td>0.10156E-01</td>
</tr>
<tr>
<td>14</td>
<td>0.18159E-02</td>
<td>0.27032E-01</td>
<td>0.33887E-01</td>
<td>0.61393E-01</td>
<td>0.72508E-02</td>
</tr>
<tr>
<td>15</td>
<td>0.10483E-02</td>
<td>0.27028E-01</td>
<td>0.34021E-01</td>
<td>0.62089E-01</td>
<td>0.50477E-02</td>
</tr>
<tr>
<td>16</td>
<td>0.59926E-03</td>
<td>0.27065E-01</td>
<td>0.34211E-01</td>
<td>0.62971E-01</td>
<td>0.34763E-02</td>
</tr>
<tr>
<td>17</td>
<td>0.39911E-03</td>
<td>0.27129E-01</td>
<td>0.34466E-01</td>
<td>0.64137E-01</td>
<td>0.23752E-02</td>
</tr>
<tr>
<td>29</td>
<td>0.73374E-07</td>
<td>0.44086E-01</td>
<td>0.86163E-01</td>
<td>0.17762</td>
<td>0.54727E-05</td>
</tr>
<tr>
<td>30</td>
<td>0.18215E-07</td>
<td>0.12471</td>
<td>0.13256</td>
<td>0.19619</td>
<td>0.16663E-05</td>
</tr>
</tbody>
</table>

**** MOLE-X-PROFILE ****

<table>
<thead>
<tr>
<th>Stage</th>
<th>Benzene</th>
<th>NAPTH</th>
<th>1:2:4-1</th>
<th>ISOPR-1</th>
<th>N-HEP-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.17282</td>
<td>0.93290E-02</td>
<td>0.16503E-01</td>
<td>0.11041E-03</td>
<td>0.24688E-02</td>
</tr>
<tr>
<td>14</td>
<td>0.17793</td>
<td>0.94925E-02</td>
<td>0.16961E-01</td>
<td>0.11636E-04</td>
<td>0.53624E-03</td>
</tr>
<tr>
<td>15</td>
<td>0.18383</td>
<td>0.96840E-02</td>
<td>0.17492E-01</td>
<td>0.11873E-05</td>
<td>0.11274E-03</td>
</tr>
<tr>
<td>16</td>
<td>0.19116</td>
<td>0.99264E-02</td>
<td>0.18154E-01</td>
<td>0.12009E-06</td>
<td>0.23468E-04</td>
</tr>
<tr>
<td>17</td>
<td>0.20054</td>
<td>0.10245E-01</td>
<td>0.19006E-01</td>
<td>0.12070E-07</td>
<td>0.48493E-05</td>
</tr>
<tr>
<td>29</td>
<td>0.49183</td>
<td>0.27647E-01</td>
<td>0.47495E-01</td>
<td>0.23868E-20</td>
<td>0.72329E-14</td>
</tr>
<tr>
<td>30</td>
<td>0.41543</td>
<td>0.26299E-01</td>
<td>0.40635E-01</td>
<td>0.10645E-21</td>
<td>0.63663E-15</td>
</tr>
<tr>
<td>Stage</td>
<td>N-HEX</td>
<td>WATER</td>
<td>H2</td>
<td>ETHYLBEN</td>
<td>TOLUENE</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>----</td>
<td>----------</td>
<td>---------</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.13023</td>
<td>0.37971E-01</td>
<td>0.13747E-03</td>
<td>0.42741E-03</td>
<td>0.62905</td>
</tr>
<tr>
<td>2</td>
<td>0.98177E-01</td>
<td>0.24228E-01</td>
<td>0.76040E-04</td>
<td>0.61334E-03</td>
<td>0.71652</td>
</tr>
<tr>
<td>10</td>
<td>0.83276E-01</td>
<td>0.22418E-01</td>
<td>0.77000E-04</td>
<td>0.15214E-02</td>
<td>0.67144</td>
</tr>
<tr>
<td>11</td>
<td>0.83329E-01</td>
<td>0.22461E-01</td>
<td>0.77219E-04</td>
<td>0.15648E-02</td>
<td>0.66165</td>
</tr>
<tr>
<td>12</td>
<td>0.82886E-01</td>
<td>0.22298E-01</td>
<td>0.36444E-04</td>
<td>0.15962E-02</td>
<td>0.65252</td>
</tr>
<tr>
<td>13</td>
<td>0.41202E-01</td>
<td>0.52434E-02</td>
<td>0.47029E-07</td>
<td>0.18828E-02</td>
<td>0.75560</td>
</tr>
<tr>
<td>14</td>
<td>0.17791E-01</td>
<td>0.10829E-02</td>
<td>0.60021E-10</td>
<td>0.20551E-02</td>
<td>0.79445</td>
</tr>
<tr>
<td>15</td>
<td>0.73336E-02</td>
<td>0.21524E-03</td>
<td>0.76602E-13</td>
<td>0.21989E-02</td>
<td>0.80626</td>
</tr>
<tr>
<td>16</td>
<td>0.29348E-02</td>
<td>0.41541E-04</td>
<td>0.96045E-16</td>
<td>0.23581E-02</td>
<td>0.80614</td>
</tr>
<tr>
<td>17</td>
<td>0.11621E-02</td>
<td>0.79447E-05</td>
<td>0.12040E-18</td>
<td>0.25515E-02</td>
<td>0.79909</td>
</tr>
<tr>
<td>29</td>
<td>0.46874E-08</td>
<td>0.41332E-14</td>
<td>0.41844E-56</td>
<td>0.88080E-02</td>
<td>0.19299</td>
</tr>
<tr>
<td>30</td>
<td>0.13373E-08</td>
<td>0.55682E-15</td>
<td>0.33293E-59</td>
<td>0.85874E-02</td>
<td>0.13343</td>
</tr>
</tbody>
</table>

**MOLE-Y-PROFILE**

<table>
<thead>
<tr>
<th>Stage</th>
<th>P-XYL</th>
<th>O-XYL</th>
<th>M-XYL</th>
<th>N-BUTANE</th>
<th>N-PENT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.18227E-01</td>
<td>0.45392E-03</td>
<td>0.15736E-02</td>
<td>0.17997E-01</td>
<td>0.89230E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.26760E-01</td>
<td>0.69918E-03</td>
<td>0.23268E-02</td>
<td>0.10709E-01</td>
<td>0.57840E-01</td>
</tr>
<tr>
<td>10</td>
<td>0.79153E-01</td>
<td>0.32436E-02</td>
<td>0.72999E-02</td>
<td>0.10344E-01</td>
<td>0.53016E-01</td>
</tr>
<tr>
<td>11</td>
<td>0.83018E-01</td>
<td>0.36016E-02</td>
<td>0.77085E-02</td>
<td>0.10370E-01</td>
<td>0.53122E-01</td>
</tr>
<tr>
<td>12</td>
<td>0.86279E-01</td>
<td>0.39606E-02</td>
<td>0.80640E-02</td>
<td>0.10261E-01</td>
<td>0.52764E-01</td>
</tr>
<tr>
<td>13</td>
<td>0.10134</td>
<td>0.46014E-02</td>
<td>0.94613E-02</td>
<td>0.12716E-02</td>
<td>0.13724E-01</td>
</tr>
<tr>
<td>14</td>
<td>0.10997</td>
<td>0.49333E-02</td>
<td>0.10251E-01</td>
<td>0.13901E-03</td>
<td>0.31083E-02</td>
</tr>
<tr>
<td>15</td>
<td>0.11688</td>
<td>0.51726E-02</td>
<td>0.10876E-01</td>
<td>0.14627E-04</td>
<td>0.67408E-03</td>
</tr>
<tr>
<td>16</td>
<td>0.12441</td>
<td>0.54216E-02</td>
<td>0.11555E-01</td>
<td>0.14919E-05</td>
<td>0.14167E-03</td>
</tr>
<tr>
<td>17</td>
<td>0.13361</td>
<td>0.57257E-02</td>
<td>0.12386E-01</td>
<td>0.15090E-06</td>
<td>0.29489E-04</td>
</tr>
<tr>
<td>29</td>
<td>0.51114</td>
<td>0.26064E-01</td>
<td>0.48832E-01</td>
<td>0.60833E-19</td>
<td>0.57983E-13</td>
</tr>
<tr>
<td>30</td>
<td>0.51294</td>
<td>0.28019E-01</td>
<td>0.49391E-01</td>
<td>0.30171E-20</td>
<td>0.90561E-14</td>
</tr>
</tbody>
</table>

**MOLE-Y-PROFILE**
### Section XII: Appendices

#### Table 1: Mole-Y-Profile

<table>
<thead>
<tr>
<th>Stage</th>
<th>Benzene</th>
<th>Napth</th>
<th>1:2:4-01</th>
<th>Isopropyl</th>
<th>N-Heptane</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.13101E-01</td>
<td>0.60558E-06</td>
<td>0.40960E-04</td>
<td>0.10128E-02</td>
<td>0.26861E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.11106E-01</td>
<td>0.12932E-05</td>
<td>0.75834E-04</td>
<td>0.16559E-02</td>
<td>0.25269E-01</td>
</tr>
<tr>
<td>10</td>
<td>0.91216E-02</td>
<td>0.37286E-03</td>
<td>0.29565E-02</td>
<td>0.14295E-01</td>
<td>0.20427E-01</td>
</tr>
<tr>
<td>11</td>
<td>0.91079E-02</td>
<td>0.75345E-03</td>
<td>0.44685E-02</td>
<td>0.17348E-01</td>
<td>0.20358E-01</td>
</tr>
<tr>
<td>12</td>
<td>0.90569E-02</td>
<td>0.15195E-02</td>
<td>0.67190E-02</td>
<td>0.20883E-01</td>
<td>0.20234E-01</td>
</tr>
<tr>
<td>13</td>
<td>0.62828E-02</td>
<td>0.17660E-02</td>
<td>0.77865E-02</td>
<td>0.24173E-01</td>
<td>0.17147E-01</td>
</tr>
<tr>
<td>14</td>
<td>0.38630E-02</td>
<td>0.18710E-02</td>
<td>0.82610E-02</td>
<td>0.25747E-01</td>
<td>0.12786E-01</td>
</tr>
<tr>
<td>15</td>
<td>0.22826E-02</td>
<td>0.19258E-02</td>
<td>0.85248E-02</td>
<td>0.26746E-01</td>
<td>0.91141E-02</td>
</tr>
<tr>
<td>16</td>
<td>0.13172E-02</td>
<td>0.19683E-02</td>
<td>0.87422E-02</td>
<td>0.27687E-01</td>
<td>0.63422E-02</td>
</tr>
<tr>
<td>17</td>
<td>0.75302E-03</td>
<td>0.20125E-02</td>
<td>0.89775E-02</td>
<td>0.28791E-01</td>
<td>0.43678E-02</td>
</tr>
<tr>
<td>29</td>
<td>0.13106E-06</td>
<td>0.12506E-01</td>
<td>0.52808E-01</td>
<td>0.14684E-01</td>
<td>0.13471E-04</td>
</tr>
<tr>
<td>30</td>
<td>0.88620E-07</td>
<td>0.21801E-01</td>
<td>0.73340E-01</td>
<td>0.17248E-01</td>
<td>0.65248E-05</td>
</tr>
</tbody>
</table>

#### Table 2: K-Values

<table>
<thead>
<tr>
<th>Stage</th>
<th>P-Xyl</th>
<th>O-Xyl</th>
<th>M-Xyl</th>
<th>N-Butane</th>
<th>N-Pent</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.30887</td>
<td>0.26061</td>
<td>0.30135</td>
<td>13.945</td>
<td>5.9813</td>
</tr>
<tr>
<td>2</td>
<td>0.38465</td>
<td>0.32491</td>
<td>0.37566</td>
<td>15.753</td>
<td>6.9298</td>
</tr>
<tr>
<td>10</td>
<td>0.45925</td>
<td>0.38957</td>
<td>0.44916</td>
<td>17.177</td>
<td>7.6996</td>
</tr>
<tr>
<td>11</td>
<td>0.46776</td>
<td>0.39700</td>
<td>0.45756</td>
<td>17.325</td>
<td>7.7812</td>
</tr>
<tr>
<td>12</td>
<td>0.44777</td>
<td>0.37967</td>
<td>0.43787</td>
<td>16.967</td>
<td>7.5835</td>
</tr>
<tr>
<td>13</td>
<td>0.55024</td>
<td>0.46748</td>
<td>0.53865</td>
<td>18.945</td>
<td>8.6726</td>
</tr>
<tr>
<td>14</td>
<td>0.58997</td>
<td>0.50144</td>
<td>0.57773</td>
<td>19.687</td>
<td>9.0836</td>
</tr>
<tr>
<td>15</td>
<td>0.60733</td>
<td>0.51627</td>
<td>0.59480</td>
<td>20.007</td>
<td>9.2606</td>
</tr>
<tr>
<td>16</td>
<td>0.61736</td>
<td>0.52489</td>
<td>0.60468</td>
<td>20.184</td>
<td>9.3584</td>
</tr>
<tr>
<td>17</td>
<td>0.62559</td>
<td>0.53203</td>
<td>0.61280</td>
<td>20.317</td>
<td>9.4334</td>
</tr>
<tr>
<td>29</td>
<td>1.0368</td>
<td>0.89563</td>
<td>1.02035</td>
<td>25.488</td>
<td>12.526</td>
</tr>
<tr>
<td>STAGE</td>
<td>N-HEX</td>
<td>WATER</td>
<td>H2</td>
<td>ETHYLBEN</td>
<td>TOLUENE</td>
</tr>
<tr>
<td>-------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>----------</td>
<td>---------</td>
</tr>
<tr>
<td>1</td>
<td>2.6536</td>
<td>6.7347</td>
<td>1681.9</td>
<td>0.33366</td>
<td>0.67948</td>
</tr>
<tr>
<td>2</td>
<td>3.1571</td>
<td>7.6447</td>
<td>1681.9</td>
<td>0.41376</td>
<td>0.82402</td>
</tr>
<tr>
<td>10</td>
<td>3.5780</td>
<td>8.6218</td>
<td>1688.7</td>
<td>0.49266</td>
<td>0.96504</td>
</tr>
<tr>
<td>11</td>
<td>3.6228</td>
<td>8.7346</td>
<td>1689.3</td>
<td>0.50165</td>
<td>0.98102</td>
</tr>
<tr>
<td>12</td>
<td>3.5127</td>
<td>8.4892</td>
<td>1720.0</td>
<td>0.48056</td>
<td>0.94377</td>
</tr>
<tr>
<td>13</td>
<td>4.1155</td>
<td>9.5987</td>
<td>1700.0</td>
<td>0.58828</td>
<td>1.1316</td>
</tr>
<tr>
<td>14</td>
<td>4.3475</td>
<td>9.9939</td>
<td>1697.3</td>
<td>0.62991</td>
<td>1.2032</td>
</tr>
<tr>
<td>15</td>
<td>4.4488</td>
<td>10.162</td>
<td>1697.7</td>
<td>0.64808</td>
<td>1.2342</td>
</tr>
<tr>
<td>16</td>
<td>4.5053</td>
<td>10.263</td>
<td>1698.1</td>
<td>0.65859</td>
<td>1.2522</td>
</tr>
<tr>
<td>17</td>
<td>4.5487</td>
<td>10.352</td>
<td>1697.9</td>
<td>0.66723</td>
<td>1.2670</td>
</tr>
<tr>
<td>29</td>
<td>6.3672</td>
<td>14.688</td>
<td>1604.0</td>
<td>1.0981</td>
<td>1.9888</td>
</tr>
<tr>
<td>30</td>
<td>7.3821</td>
<td>16.100</td>
<td>1638.9</td>
<td>1.3028</td>
<td>2.3171</td>
</tr>
</tbody>
</table>

*** K-VALUES ***

<table>
<thead>
<tr>
<th>STAGE</th>
<th>BENZENE</th>
<th>NAPTH</th>
<th>1:2:4-01</th>
<th>ISOPR-01</th>
<th>N-HEP-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.6979</td>
<td>0.30463E-01</td>
<td>0.11400</td>
<td>0.20702</td>
<td>1.2064</td>
</tr>
<tr>
<td>2</td>
<td>1.9952</td>
<td>0.39677E-01</td>
<td>0.14631</td>
<td>0.26078</td>
<td>1.4741</td>
</tr>
<tr>
<td>10</td>
<td>2.2868</td>
<td>0.49918E-01</td>
<td>0.17909</td>
<td>0.31332</td>
<td>1.7024</td>
</tr>
<tr>
<td>11</td>
<td>2.3199</td>
<td>0.51146E-01</td>
<td>0.18288</td>
<td>0.31931</td>
<td>1.7269</td>
</tr>
<tr>
<td>12</td>
<td>2.2465</td>
<td>0.48335E-01</td>
<td>0.17397</td>
<td>0.30514</td>
<td>1.6657</td>
</tr>
<tr>
<td>13</td>
<td>2.6188</td>
<td>0.62262E-01</td>
<td>0.21998</td>
<td>0.37877</td>
<td>1.9994</td>
</tr>
<tr>
<td>14</td>
<td>2.7575</td>
<td>0.67747E-01</td>
<td>0.23814</td>
<td>0.40759</td>
<td>2.1300</td>
</tr>
<tr>
<td>15</td>
<td>2.8174</td>
<td>0.70158E-01</td>
<td>0.24613</td>
<td>0.42022</td>
<td>2.1872</td>
</tr>
<tr>
<td>16</td>
<td>2.8523</td>
<td>0.71588E-01</td>
<td>0.25076</td>
<td>0.42750</td>
<td>2.2191</td>
</tr>
<tr>
<td>17</td>
<td>2.8814</td>
<td>0.72812E-01</td>
<td>0.25458</td>
<td>0.43343</td>
<td>2.2436</td>
</tr>
<tr>
<td>29</td>
<td>4.2714</td>
<td>0.14310</td>
<td>0.45402</td>
<td>0.73044</td>
<td>3.3077</td>
</tr>
<tr>
<td>30</td>
<td>4.8653</td>
<td>0.17482</td>
<td>0.55326</td>
<td>0.87918</td>
<td>3.9156</td>
</tr>
</tbody>
</table>

*** K-VALUES ***

<table>
<thead>
<tr>
<th>STAGE</th>
<th>1-BUT-01</th>
<th>1-PEN-01</th>
<th>1-HEX-01</th>
<th>1-HEP-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>15.612</td>
<td>6.7087</td>
<td>2.9460</td>
<td>1.3054</td>
</tr>
<tr>
<td>2</td>
<td>17.565</td>
<td>7.7389</td>
<td>3.4849</td>
<td>1.5857</td>
</tr>
<tr>
<td>10</td>
<td>19.111</td>
<td>8.5842</td>
<td>3.9403</td>
<td>1.8293</td>
</tr>
<tr>
<td>11</td>
<td>19.272</td>
<td>8.6736</td>
<td>3.9891</td>
<td>1.8557</td>
</tr>
<tr>
<td>12</td>
<td>18.883</td>
<td>8.4567</td>
<td>3.8703</td>
<td>1.7912</td>
</tr>
<tr>
<td>13</td>
<td>21.012</td>
<td>9.6331</td>
<td>4.5135</td>
<td>2.1412</td>
</tr>
<tr>
<td>14</td>
<td>21.805</td>
<td>10.077</td>
<td>4.7592</td>
<td>2.2769</td>
</tr>
<tr>
<td>15</td>
<td>22.146</td>
<td>10.268</td>
<td>4.8659</td>
<td>2.3362</td>
</tr>
<tr>
<td>Stage</td>
<td>Benzene</td>
<td>Napth 1:2:4-01</td>
<td>Isopr-01</td>
<td>N-Hept-01</td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>----------------</td>
<td>----------</td>
<td>-----------</td>
</tr>
<tr>
<td>1</td>
<td>0.73789E-02</td>
<td>0.30035E-05</td>
<td>0.15631E-03</td>
<td>0.32210E-02</td>
</tr>
<tr>
<td>2</td>
<td>0.50925E-02</td>
<td>0.72313E-05</td>
<td>0.30651E-03</td>
<td>0.53353E-02</td>
</tr>
<tr>
<td>10</td>
<td>0.32568E-02</td>
<td>0.22987E-02</td>
<td>0.12724E-01</td>
<td>0.48028E-01</td>
</tr>
<tr>
<td>11</td>
<td>0.31977E-02</td>
<td>0.45772E-02</td>
<td>0.18919E-01</td>
<td>0.57404E-01</td>
</tr>
<tr>
<td>12</td>
<td>0.39659E-02</td>
<td>0.36173E-01</td>
<td>0.41796E-01</td>
<td>0.74144E-01</td>
</tr>
</tbody>
</table>

** **** MASS-X-PROFILE ****

<table>
<thead>
<tr>
<th>Stage</th>
<th>P-XYL</th>
<th>O-XYL</th>
<th>M-XYL</th>
<th>N-Butane</th>
<th>N-Pent</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.43307E-01</td>
<td>0.11635E-02</td>
<td>0.37817E-02</td>
<td>0.10811E-02</td>
<td>0.15022E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.62106E-01</td>
<td>0.17822E-02</td>
<td>0.54745E-02</td>
<td>0.44198E-03</td>
<td>0.69235E-02</td>
</tr>
<tr>
<td>10</td>
<td>0.18401E+00</td>
<td>0.84613E-02</td>
<td>0.17255E-01</td>
<td>0.36474E-03</td>
<td>0.51792E-02</td>
</tr>
<tr>
<td>11</td>
<td>0.18991E+00</td>
<td>0.92515E-02</td>
<td>0.17931E-01</td>
<td>0.36267E-03</td>
<td>0.51341E-02</td>
</tr>
<tr>
<td>12</td>
<td>0.18171E+00</td>
<td>0.99467E-02</td>
<td>0.17387E-01</td>
<td>0.59725E-03</td>
<td>0.80016E-02</td>
</tr>
<tr>
<td>13</td>
<td>0.18640E+00</td>
<td>0.10062E-01</td>
<td>0.17800E-01</td>
<td>0.65199E-04</td>
<td>0.18097E-02</td>
</tr>
<tr>
<td>14</td>
<td>0.19144E+00</td>
<td>0.10214E-01</td>
<td>0.18250E-01</td>
<td>0.68545E-05</td>
<td>0.39211E-03</td>
</tr>
<tr>
<td>15</td>
<td>0.19749E+00</td>
<td>0.10404E-01</td>
<td>0.18792E-01</td>
<td>0.69833E-06</td>
<td>0.82312E-04</td>
</tr>
<tr>
<td>16</td>
<td>0.20504E+00</td>
<td>0.10647E-01</td>
<td>0.19473E-01</td>
<td>0.70520E-07</td>
<td>0.17107E-04</td>
</tr>
<tr>
<td>17</td>
<td>0.21469E+00</td>
<td>0.10968E-01</td>
<td>0.20347E-01</td>
<td>0.70742E-08</td>
<td>0.35281E-05</td>
</tr>
<tr>
<td>29</td>
<td>0.47818E+00</td>
<td>0.26880E-01</td>
<td>0.46178E-01</td>
<td>0.12704E-20</td>
<td>0.47790E-14</td>
</tr>
<tr>
<td>30</td>
<td>0.39130E+00</td>
<td>0.24771E-01</td>
<td>0.38275E-01</td>
<td>0.54894E-22</td>
<td>0.40751E-15</td>
</tr>
</tbody>
</table>

** **** MASS-X-PROFILE ****

<table>
<thead>
<tr>
<th>Stage</th>
<th>N-Hex</th>
<th>Water</th>
<th>H2</th>
<th>Ethylben</th>
<th>Toluene</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.55183E-01</td>
<td>0.14264E-02</td>
<td>0.24341E-08</td>
<td>0.97875E-03</td>
<td>0.83078</td>
</tr>
<tr>
<td>2</td>
<td>0.31566E-01</td>
<td>0.65313E-03</td>
<td>0.98776E-09</td>
<td>0.13631E-02</td>
<td>0.85259</td>
</tr>
<tr>
<td>10</td>
<td>0.20932E-01</td>
<td>0.48837E-03</td>
<td>0.95763E-09</td>
<td>0.33495E-02</td>
<td>0.67671</td>
</tr>
<tr>
<td>11</td>
<td>0.20659E-01</td>
<td>0.48292E-03</td>
<td>0.96081E-09</td>
<td>0.33876E-02</td>
<td>0.65217</td>
</tr>
<tr>
<td>12</td>
<td>0.28693E-01</td>
<td>0.76334E-03</td>
<td>0.76612E-09</td>
<td>0.31188E-02</td>
<td>0.57401</td>
</tr>
<tr>
<td>13</td>
<td>0.12372E-01</td>
<td>0.15743E-03</td>
<td>0.97636E-12</td>
<td>0.32233E-02</td>
<td>0.60178</td>
</tr>
<tr>
<td>14</td>
<td>0.50953E-02</td>
<td>0.31263E-04</td>
<td>0.12450E-14</td>
<td>0.33324E-02</td>
<td>0.60994</td>
</tr>
<tr>
<td>15</td>
<td>0.20367E-02</td>
<td>0.60267E-05</td>
<td>0.15592E-17</td>
<td>0.34618E-02</td>
<td>0.60913</td>
</tr>
<tr>
<td>16</td>
<td>0.80520E-03</td>
<td>0.11508E-05</td>
<td>0.19514E-20</td>
<td>0.36216E-02</td>
<td>0.60294</td>
</tr>
<tr>
<td>17</td>
<td>0.31567E-03</td>
<td>0.21792E-06</td>
<td>0.14414E-23</td>
<td>0.38225E-02</td>
<td>0.59237</td>
</tr>
<tr>
<td>29</td>
<td>0.85781E-09</td>
<td>0.73206E-16</td>
<td>0.48161E-61</td>
<td>0.79289E-02</td>
<td>0.98729E-01</td>
</tr>
<tr>
<td>30</td>
<td>0.13850E-09</td>
<td>0.55277E-17</td>
<td>0.36331E-64</td>
<td>0.62084E-02</td>
<td>0.47073E-01</td>
</tr>
<tr>
<td>STAGE</td>
<td>1-BUT-01</td>
<td>1-PEN-01</td>
<td>1-HEX-01</td>
<td>1-HEP-01</td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td>---------</td>
<td></td>
</tr>
<tr>
<td>0.14312E-03</td>
<td>0.16183E-02</td>
<td>0.62132E-02</td>
<td>0.30121E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.57990E-04</td>
<td>0.73025E-03</td>
<td>0.34425E-02</td>
<td>0.22707E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.48327E-04</td>
<td>0.55440E-03</td>
<td>0.23175E-02</td>
<td>0.14331E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.48065E-04</td>
<td>0.54978E-03</td>
<td>0.22885E-02</td>
<td>0.14043E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.79481E-04</td>
<td>0.86617E-03</td>
<td>0.32402E-02</td>
<td>0.16230E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.78586E-05</td>
<td>0.17806E-03</td>
<td>0.12946E-02</td>
<td>0.11524E-02</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.74916E-06</td>
<td>0.35093E-04</td>
<td>0.49447E-03</td>
<td>0.78294E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.69232E-07</td>
<td>0.67003E-05</td>
<td>0.18328E-03</td>
<td>0.51895E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.63433E-08</td>
<td>0.12667E-05</td>
<td>0.67210E-04</td>
<td>0.34031E-03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.57743E-09</td>
<td>0.23764E-06</td>
<td>0.24442E-04</td>
<td>0.22130E-03</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**** MASS-Y-PROFILE ***

<table>
<thead>
<tr>
<th>STAGE</th>
<th>P-XYL</th>
<th>O-XYL</th>
<th>M-XYL</th>
<th>N-BUTANE</th>
<th>N-PENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.22491E-01</td>
<td>0.56010E-03</td>
<td>0.19416E-02</td>
<td>0.12157E-01</td>
<td>0.74825E-01</td>
<td></td>
</tr>
<tr>
<td>0.32115E-01</td>
<td>0.83911E-03</td>
<td>0.27924E-02</td>
<td>0.70361E-02</td>
<td>0.47174E-01</td>
<td></td>
</tr>
<tr>
<td>0.93258E-01</td>
<td>0.38217E-02</td>
<td>0.86008E-02</td>
<td>0.66719E-02</td>
<td>0.42450E-01</td>
<td></td>
</tr>
<tr>
<td>0.97596E-01</td>
<td>0.42340E-02</td>
<td>0.90620E-02</td>
<td>0.66740E-02</td>
<td>0.42441E-01</td>
<td></td>
</tr>
<tr>
<td>0.10112</td>
<td>0.46419E-02</td>
<td>0.94510E-02</td>
<td>0.65839E-02</td>
<td>0.42025E-01</td>
<td></td>
</tr>
<tr>
<td>0.11473</td>
<td>0.52093E-02</td>
<td>0.10711E-01</td>
<td>0.78811E-03</td>
<td>0.10559E-01</td>
<td></td>
</tr>
<tr>
<td>0.12325</td>
<td>0.55290E-02</td>
<td>0.11489E-01</td>
<td>0.85295E-04</td>
<td>0.23675E-02</td>
<td></td>
</tr>
<tr>
<td>0.13053</td>
<td>0.57769E-02</td>
<td>0.12147E-01</td>
<td>0.89435E-05</td>
<td>0.51162E-03</td>
<td></td>
</tr>
<tr>
<td>0.13865</td>
<td>0.60423E-02</td>
<td>0.12878E-01</td>
<td>0.91030E-06</td>
<td>0.10730E-03</td>
<td></td>
</tr>
<tr>
<td>0.14861</td>
<td>0.63682E-02</td>
<td>0.13776E-01</td>
<td>0.91885E-07</td>
<td>0.22289E-04</td>
<td></td>
</tr>
<tr>
<td>0.50937</td>
<td>0.25974E-01</td>
<td>0.48663E-01</td>
<td>0.33189E-19</td>
<td>0.39268E-13</td>
<td></td>
</tr>
<tr>
<td>0.50320</td>
<td>0.27487E-01</td>
<td>0.48453E-01</td>
<td>0.16204E-20</td>
<td>0.60375E-14</td>
<td></td>
</tr>
</tbody>
</table>

**** MASS-Y-PROFILE ***

<table>
<thead>
<tr>
<th>STAGE</th>
<th>N-HEX</th>
<th>WATER</th>
<th>H2</th>
<th>ETHYLBEN</th>
<th>TOLUENE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.13043</td>
<td>0.79503E-02</td>
<td>0.32209E-05</td>
<td>0.52739E-03</td>
<td>0.67364</td>
<td></td>
</tr>
<tr>
<td>0.95639E-01</td>
<td>0.49339E-02</td>
<td>0.17328E-05</td>
<td>0.73608E-03</td>
<td>0.74630</td>
<td></td>
</tr>
</tbody>
</table>

476
<table>
<thead>
<tr>
<th>Stage</th>
<th>Benzene</th>
<th>Naph</th>
<th>1:2:4-1</th>
<th>Isoprop</th>
<th>N-Heptane</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.11894E-01</td>
<td>0.90212E-06</td>
<td>0.57219E-04</td>
<td>0.14148E-02</td>
<td>0.31282E-01</td>
</tr>
<tr>
<td>2</td>
<td>0.98065E-02</td>
<td>0.18737E-05</td>
<td>0.10304E-03</td>
<td>0.22499E-02</td>
<td>0.28623E-01</td>
</tr>
<tr>
<td>10</td>
<td>0.79073E-02</td>
<td>0.53036E-03</td>
<td>0.39435E-02</td>
<td>0.19067E-01</td>
<td>0.22716E-01</td>
</tr>
<tr>
<td>11</td>
<td>0.78779E-02</td>
<td>0.10693E-02</td>
<td>0.59472E-02</td>
<td>0.23089E-01</td>
<td>0.22589E-01</td>
</tr>
<tr>
<td>12</td>
<td>0.78098E-02</td>
<td>0.21500E-02</td>
<td>0.89151E-02</td>
<td>0.27708E-01</td>
<td>0.22382E-01</td>
</tr>
<tr>
<td>13</td>
<td>0.52333E-02</td>
<td>0.24137E-02</td>
<td>0.99798E-02</td>
<td>0.30983E-01</td>
<td>0.18322E-01</td>
</tr>
<tr>
<td>14</td>
<td>0.31854E-02</td>
<td>0.25316E-02</td>
<td>0.10482E-01</td>
<td>0.32668E-01</td>
<td>0.13525E-01</td>
</tr>
<tr>
<td>15</td>
<td>0.18757E-02</td>
<td>0.25965E-02</td>
<td>0.10779E-01</td>
<td>0.33817E-01</td>
<td>0.96072E-02</td>
</tr>
<tr>
<td>16</td>
<td>0.10801E-02</td>
<td>0.26483E-02</td>
<td>0.11030E-01</td>
<td>0.34934E-01</td>
<td>0.66713E-02</td>
</tr>
<tr>
<td>17</td>
<td>0.61621E-03</td>
<td>0.27023E-02</td>
<td>0.11304E-01</td>
<td>0.36253E-01</td>
<td>0.45851E-02</td>
</tr>
<tr>
<td>29</td>
<td>0.16387E-06</td>
<td>0.15046E-01</td>
<td>0.59578E-01</td>
<td>0.16566</td>
<td>0.12671E-04</td>
</tr>
<tr>
<td>30</td>
<td>0.63964E-07</td>
<td>0.25820E-01</td>
<td>0.81452E-01</td>
<td>0.19156</td>
<td>0.60413E-05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stage</th>
<th>1-Butanol</th>
<th>1-Phenol</th>
<th>1-Hexanol</th>
<th>1-Heptane</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.17970E-02</td>
<td>0.89867E-02</td>
<td>0.16115E-01</td>
<td>0.39253E-02</td>
</tr>
<tr>
<td>2</td>
<td>0.10323E-02</td>
<td>0.55798E-02</td>
<td>0.11537E-01</td>
<td>0.35031E-02</td>
</tr>
<tr>
<td>10</td>
<td>0.98357E-03</td>
<td>0.50664E-02</td>
<td>0.97123E-02</td>
<td>0.27805E-02</td>
</tr>
<tr>
<td>11</td>
<td>0.98391E-03</td>
<td>0.50658E-02</td>
<td>0.96992E-02</td>
<td>0.27664E-02</td>
</tr>
<tr>
<td>12</td>
<td>0.96988E-03</td>
<td>0.50145E-02</td>
<td>0.96171E-02</td>
<td>0.27417E-02</td>
</tr>
<tr>
<td>13</td>
<td>0.10488E-03</td>
<td>0.11430E-02</td>
<td>0.42756E-02</td>
<td>0.21417E-02</td>
</tr>
<tr>
<td>14</td>
<td>0.10281E-04</td>
<td>0.23293E-03</td>
<td>0.16936E-02</td>
<td>0.15075E-02</td>
</tr>
<tr>
<td>15</td>
<td>0.97748E-06</td>
<td>0.45788E-04</td>
<td>0.64517E-03</td>
<td>0.10215E-02</td>
</tr>
<tr>
<td>16</td>
<td>0.90248E-07</td>
<td>0.87342E-05</td>
<td>0.23892E-03</td>
<td>0.67646E-03</td>
</tr>
<tr>
<td>17</td>
<td>0.82652E-08</td>
<td>0.16504E-05</td>
<td>0.87572E-04</td>
<td>0.44339E-03</td>
</tr>
<tr>
<td>29</td>
<td>0.58304E-21</td>
<td>0.94057E-15</td>
<td>0.12743E-09</td>
<td>0.67472E-06</td>
</tr>
<tr>
<td>30</td>
<td>0.25880E-22</td>
<td>0.13219E-15</td>
<td>0.33242E-10</td>
<td>0.30550E-06</td>
</tr>
</tbody>
</table>

**** MURPHREE EFF ****
<table>
<thead>
<tr>
<th>STAGE</th>
<th>P-XYL</th>
<th>O-XYL</th>
<th>M-XYL</th>
<th>N-BUTANE</th>
<th>N-PENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>2</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>10</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>11</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>12</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>13</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>14</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>15</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>16</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>17</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>29</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
<tr>
<td>30</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
</tbody>
</table>

**** MURPHREE EFF ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>N-HEX</th>
<th>WATER</th>
<th>H2</th>
<th>ETHYLBEN</th>
<th>TOLUENE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>2</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>10</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>11</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>12</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>13</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>14</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>15</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>16</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>17</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>29</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
<tr>
<td>30</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
</tbody>
</table>

**** MURPHREE EFF ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>BENZENE</th>
<th>NAPTH</th>
<th>1:2:4-01</th>
<th>ISOPR-01</th>
<th>N-HEP-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>2</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>10</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>11</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>12</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>13</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>14</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>15</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>16</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>17</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>29</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
<tr>
<td>30</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
</tbody>
</table>
**** MURPHREE EFF ****

<table>
<thead>
<tr>
<th></th>
<th>1-BUT-01</th>
<th>1-PEN-01</th>
<th>1-HEX-01</th>
<th>1-HEP-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>2</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
<td>0.56000</td>
</tr>
<tr>
<td>10</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>11</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>12</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
<td>0.57000</td>
</tr>
<tr>
<td>13</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>14</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
<td>0.58000</td>
</tr>
<tr>
<td>15</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>16</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>17</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
<td>0.59000</td>
</tr>
<tr>
<td>29</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
<tr>
<td>30</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
<td>0.60000</td>
</tr>
</tbody>
</table>

****************************
***** HYDRAULIC PARAMETERS *****
****************************

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)

WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

TEMPERATURE
### Stage 1: Liquid from Vapor to Liquid

<table>
<thead>
<tr>
<th>Stage</th>
<th>Mass Flow (LB/HR)</th>
<th>Volume Flow (CUFT/HR)</th>
<th>Molecular Weight</th>
<th>Density (LB/CUFT)</th>
<th>Viscosity (CP)</th>
<th>Surface Tension (Dyne/CM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.8484E+06</td>
<td>0.39976E+06</td>
<td>3863.6</td>
<td>47.841</td>
<td>0.18404</td>
<td>0.25600</td>
</tr>
<tr>
<td>2</td>
<td>1.8809E+06</td>
<td>0.40302E+06</td>
<td>3912.9</td>
<td>48.070</td>
<td>0.18418</td>
<td>0.24808</td>
</tr>
<tr>
<td>10</td>
<td>1.8679E+06</td>
<td>0.40172E+06</td>
<td>3885.7</td>
<td>48.072</td>
<td>0.18475</td>
<td>0.24473</td>
</tr>
<tr>
<td>11</td>
<td>1.9023E+06</td>
<td>0.40516E+06</td>
<td>3957.1</td>
<td>48.074</td>
<td>0.18609</td>
<td>0.24497</td>
</tr>
<tr>
<td>12</td>
<td>5.9165E+06</td>
<td>0.44836E+06</td>
<td>12254.0</td>
<td>48.280</td>
<td>0.18936</td>
<td>0.25370</td>
</tr>
<tr>
<td>13</td>
<td>6.0817E+06</td>
<td>0.46489E+06</td>
<td>12587.0</td>
<td>48.895</td>
<td>0.19034</td>
<td>0.25600</td>
</tr>
<tr>
<td>14</td>
<td>6.1342E+06</td>
<td>0.47014E+06</td>
<td>12682.0</td>
<td>49.000</td>
<td>0.19169</td>
<td>0.25700</td>
</tr>
<tr>
<td>15</td>
<td>6.1531E+06</td>
<td>0.47203E+06</td>
<td>12731.0</td>
<td>49.000</td>
<td>0.19205</td>
<td>0.25752</td>
</tr>
<tr>
<td>16</td>
<td>6.1622E+06</td>
<td>0.47294E+06</td>
<td>12784.0</td>
<td>49.000</td>
<td>0.19240</td>
<td>0.25803</td>
</tr>
<tr>
<td>17</td>
<td>6.1689E+06</td>
<td>0.47360E+06</td>
<td>12787.0</td>
<td>49.000</td>
<td>0.19275</td>
<td>0.25854</td>
</tr>
<tr>
<td>29</td>
<td>0.64102E+06</td>
<td>0.49774E+06</td>
<td>13446.0</td>
<td>50.000</td>
<td>0.19500</td>
<td>0.26100</td>
</tr>
<tr>
<td>30</td>
<td>0.14328E+06</td>
<td>0.0000</td>
<td>2969.4</td>
<td>50.000</td>
<td>0.19535</td>
<td>0.26150</td>
</tr>
</tbody>
</table>

### Stage 2: Liquid from Vapor to Liquid

<table>
<thead>
<tr>
<th>Stage</th>
<th>Mass Flow (LB/HR)</th>
<th>Volume Flow (CUFT/HR)</th>
<th>Molecular Weight</th>
<th>Density (LB/CUFT)</th>
<th>Viscosity (CP)</th>
<th>Surface Tension (Dyne/CM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>209.00</td>
<td>221.14</td>
<td>3863.6</td>
<td>47.841</td>
<td>0.18404</td>
<td>0.25600</td>
</tr>
<tr>
<td>2</td>
<td>221.14</td>
<td>224.21</td>
<td>3912.9</td>
<td>48.070</td>
<td>0.18418</td>
<td>0.24808</td>
</tr>
<tr>
<td>10</td>
<td>231.40</td>
<td>229.90</td>
<td>3885.7</td>
<td>48.072</td>
<td>0.18475</td>
<td>0.24473</td>
</tr>
<tr>
<td>11</td>
<td>232.48</td>
<td>229.92</td>
<td>3957.1</td>
<td>48.074</td>
<td>0.18609</td>
<td>0.24497</td>
</tr>
<tr>
<td>12</td>
<td>242.19</td>
<td>246.46</td>
<td>40516.0</td>
<td>48.280</td>
<td>0.18936</td>
<td>0.25370</td>
</tr>
<tr>
<td>13</td>
<td>248.25</td>
<td>249.27</td>
<td>42036.0</td>
<td>48.895</td>
<td>0.19034</td>
<td>0.25600</td>
</tr>
<tr>
<td>14</td>
<td>246.46</td>
<td>248.25</td>
<td>44836.0</td>
<td>49.000</td>
<td>0.19169</td>
<td>0.25700</td>
</tr>
<tr>
<td>15</td>
<td>249.27</td>
<td>250.10</td>
<td>46489.0</td>
<td>49.000</td>
<td>0.19205</td>
<td>0.25752</td>
</tr>
<tr>
<td>16</td>
<td>250.10</td>
<td>251.00</td>
<td>47014.0</td>
<td>49.000</td>
<td>0.19240</td>
<td>0.25803</td>
</tr>
<tr>
<td>17</td>
<td>251.00</td>
<td>251.00</td>
<td>47203.0</td>
<td>49.000</td>
<td>0.19275</td>
<td>0.25854</td>
</tr>
<tr>
<td>29</td>
<td>283.89</td>
<td>296.36</td>
<td>49774.0</td>
<td>50.000</td>
<td>0.19500</td>
<td>0.26100</td>
</tr>
<tr>
<td>30</td>
<td>296.36</td>
<td>296.36</td>
<td>50000.0</td>
<td>50.000</td>
<td>0.19535</td>
<td>0.26150</td>
</tr>
<tr>
<td></td>
<td>MARANGONI INDEX</td>
<td>FLOW PARAM</td>
<td>QR</td>
<td>REDUCED F-FACTOR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>----------------</td>
<td>------------</td>
<td>----</td>
<td>-----------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>STAGE</td>
<td>DYNE/CM</td>
<td>CUFT/HR</td>
<td>(LB-CUFT)**.5/HR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.28678E-01</td>
<td>0.13499E+06</td>
<td>0.93186E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-8.4704E-01</td>
<td>0.28889E-01</td>
<td>0.13571E+06</td>
<td>0.93910E+06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.32782E-02</td>
<td>0.28826E-01</td>
<td>0.13506E+06</td>
<td>0.93461E+06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.11486E-01</td>
<td>0.29212E-01</td>
<td>0.13572E+06</td>
<td>0.93922E+06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>-9.5596</td>
<td>0.82641E-01</td>
<td>0.14858E+06</td>
<td>0.10303E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>-3.5356</td>
<td>0.82065E-01</td>
<td>0.15368E+06</td>
<td>0.10662E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>-8.7506E-01</td>
<td>0.81844E-01</td>
<td>0.15526E+06</td>
<td>0.10777E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>-2.0246E-01</td>
<td>0.81766E-01</td>
<td>0.15578E+06</td>
<td>0.10817E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>-5.6825E-02</td>
<td>0.81755E-01</td>
<td>0.15599E+06</td>
<td>0.10833E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>-4.7522E-02</td>
<td>0.81781E-01</td>
<td>0.15611E+06</td>
<td>0.10841E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>-8.0505E-01</td>
<td>0.84105E-01</td>
<td>0.16021E+06</td>
<td>0.11038E+07</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.53402</td>
<td>0.0000</td>
<td>0.0000</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

****** TRAY SIZING CALCULATIONS *****

*** SECTION 1 ***

STARTING STAGE NUMBER 2
ENDING STAGE NUMBER 13
FLOODING CALCULATION METHOD GLITSCH

DESIGN PARAMETERS
Castillo, Ernst, Lerch, Winchester

PEAK CAPACITY FACTOR  1.00000
SYSTEM FOAMING FACTOR  1.00000
FLOODING FACTOR  0.80000
MINIMUM COLUMN DIAMETER  FT  1.00000
MINIMUM DC AREA/COLUMN AREA  0.100000
HOLE AREA/ACTIVE AREA  0.12000

TRAY SPECIFICATIONS
-------------------
TRAY TYPE  SIEVE
NUMBER OF PASSES  1
TRAY SPACING  FT  2.00000

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER  13
COLUMN DIAMETER  FT  16.0155
DC AREA/COLUMN AREA  0.100000
DOWNCOMER VELOCITY  FT/SEC  0.17356
FLOW PATH LENGTH  FT  11.0034
SIDE DOWNCOMER WIDTH  FT  2.50603
SIDE WEIR LENGTH  FT  11.6370
CENTER DOWNCOMER WIDTH  FT  0.0
CENTER WEIR LENGTH  FT  0.0
OFF-CENTER DOWNCOMER WIDTH  FT  0.0
OFF-CENTER SHORT WEIR LENGTH  FT  0.0
OFF-CENTER LONG WEIR LENGTH  FT  0.0
TRAY CENTER TO OCDC CENTER  FT  0.0

**** SIZING PROFILES ****

<table>
<thead>
<tr>
<th>STAGE</th>
<th>DIAMETER</th>
<th>TOTAL AREA</th>
<th>ACTIVE AREA</th>
<th>SIDE DC AREA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FT</td>
<td>SQFT</td>
<td>SQFT</td>
<td>SQFT</td>
</tr>
<tr>
<td>2</td>
<td>13.535</td>
<td>143.89</td>
<td>115.11</td>
<td>14.389</td>
</tr>
<tr>
<td>3</td>
<td>13.535</td>
<td>143.89</td>
<td>115.11</td>
<td>14.389</td>
</tr>
<tr>
<td>4</td>
<td>13.531</td>
<td>143.79</td>
<td>115.03</td>
<td>14.379</td>
</tr>
<tr>
<td>5</td>
<td>13.526</td>
<td>143.69</td>
<td>114.95</td>
<td>14.369</td>
</tr>
<tr>
<td>6</td>
<td>13.522</td>
<td>143.60</td>
<td>114.88</td>
<td>14.360</td>
</tr>
<tr>
<td>7</td>
<td>13.517</td>
<td>143.49</td>
<td>114.80</td>
<td>14.349</td>
</tr>
<tr>
<td>8</td>
<td>13.512</td>
<td>143.39</td>
<td>114.71</td>
<td>14.339</td>
</tr>
</tbody>
</table>
Section XII: Appendices

9  13.506  143.26  114.61  14.326  
10  13.500  143.13  114.51  14.313  
11  13.544  144.08  115.27  14.408  
12  15.722  194.15  155.32  19.415  
13  16.015  201.45  161.16  20.145  

**BLOCK: F-300  MODEL: FLASH2**

-----------------------------
INLET STREAM:   S-307
OUTLET VAPOR STREAM:   S-310
OUTLET LIQUID STREAM:   S-308
PROPERTY OPTION SET:   PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BALANCE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>15947.6</td>
<td>15947.6</td>
</tr>
<tr>
<td>MASS(LB/HR)</td>
<td>339324.</td>
<td>339324.</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.155911E+10</td>
<td>-0.148209E+10</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E  93768.7  LB/HR
PRODUCT STREAMS CO2E  93768.7  LB/HR
NET STREAMS CO2E PRODUCTION  0.00000  LB/HR
UTILITIES CO2E PRODUCTION  0.00000  LB/HR
TOTAL CO2E PRODUCTION  0.00000  LB/HR

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE F  359.600
SPECIFIED PRESSURE  PSIA  290.075
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE  0.000100000

*** RESULTS ***

OUTLET TEMPERATURE  F  359.60
OUTLET PRESSURE  PSIA  290.08
HEAT DUTY  BTU/HR  0.77018E+08
VAPOR FRACTION  0.82624
CASTILLO, ERNST, LERCH, WINCHESTER

V-L PHASE EQUILIBRIUM:

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SORBITOL</td>
<td>0.14845E-01</td>
<td>0.85434E-01</td>
<td>0.15889E-06</td>
<td>0.18599E-05</td>
</tr>
<tr>
<td>PROPANE</td>
<td>0.40088E-01</td>
<td>0.11061E-03</td>
<td>0.48495E-01</td>
<td>438.45</td>
</tr>
<tr>
<td>CO2</td>
<td>0.13360</td>
<td>0.73119E-03</td>
<td>0.16154</td>
<td>220.93</td>
</tr>
<tr>
<td>WATER</td>
<td>0.58063</td>
<td>0.91363</td>
<td>0.51060</td>
<td>0.55887</td>
</tr>
<tr>
<td>H2</td>
<td>0.23084</td>
<td>0.97993E-04</td>
<td>0.27936</td>
<td>2850.8</td>
</tr>
</tbody>
</table>

**BLOCK: HX-100**  **MODEL: HEATX**

-----------------------------
**HOT SIDE:**
-----------------------------
**INLET STREAM:** S-417
**OUTLET STREAM:** S-420
**PROPERTY OPTION SET:** PENG-ROB STANDARD PR EQUATION OF STATE

-----------------------------
**COLD SIDE:**
-----------------------------
**INLET STREAM:** S-104
**OUTLET STREAM:** S-107
**PROPERTY OPTION SET:** PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>27662.9</td>
<td>27662.9</td>
<td>0.00000</td>
</tr>
<tr>
<td>MASS(LB/HR   )</td>
<td>748975</td>
<td>748975</td>
<td>0.155433E-15</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.337380E+10</td>
<td>-0.337380E+10</td>
<td>-0.424006E-15</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

| FEED STREAMS CO2E | 0.00000 | LB/HR |
| PRODUCT STREAMS CO2E | 0.00000 | LB/HR |
| NET STREAMS CO2E PRODUCTION | 0.00000 | LB/HR |
| UTILITIES CO2E PRODUCTION | 0.00000 | LB/HR |
| TOTAL CO2E PRODUCTION | 0.00000 | LB/HR |

*** INPUT DATA ***

FLASH SPECS FOR HOT SIDE:
**TWO PHASE FLASH**
**MAXIMUM NO. ITERATIONS** 30
**CONVERGENCE TOLERANCE** 0.000100000
FLASH SPECS FOR COLD SIDE:
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.00010000

FLOW DIRECTION AND SPECIFICATION:
COUNTERCURRENT HEAT EXCHANGER
SPECIFIED COLD OUTLET TEMP
SPECIFIED VALUE F 212.0000
LMTD CORRECTION FACTOR 1.00000

PRESSURE SPECIFICATION:
HOT SIDE PRESSURE DROP PSI 0.0000
COLD SIDE PRESSURE DROP PSI 0.0000

HEAT TRANSFER COEFFICIENT SPECIFICATION:
OVERALL COEFFICIENT BTU/HR-SQFT-R 50.0000

*** OVERALL RESULTS ***

STREAMS:

| S-417 ----->| HOT |-----> S-420
T= 6.9800D+02 | T= 5.0598D+02
P= 6.3970D+02 | P= 6.3970D+02
V= 1.0000D+00 | V= 1.0000D+00

| S-107 <-----| COLD |<----- S-104
T= 2.1200D+02 | T= 7.7042D+01
P= 4.2414D+01 | P= 4.2414D+01
V= 0.0000D+00 | V= 0.0000D+00

DUTY AND AREA:
CALCULATED HEAT DUTY BTU/HR 36902766.2465
CALCULATED (REQUIRED) AREA SQFT 1615.4392
ACTUAL EXCHANGER AREA SQFT 1615.4392
PER CENT OVER-DESIGN 0.0000

HEAT TRANSFER COEFFICIENT:
Castillo, Ernst, Lerch, Winchester

AVERAGE COEFFICIENT (DIRTY) BTU/HR-SQFT-R 50.0000
UA (DIRTY) BTU/HR-R 80771.9596

LOG-MEAN TEMPERATURE DIFFERENCE:
LMTD CORRECTION FACTOR 1.0000
LMTD (CORRECTED) F 456.8760
NUMBER OF SHELLS IN SERIES 1

PRESSURE DROP:
HOTSIDE, TOTAL PSI 0.0000
COLDSIDE, TOTAL PSI 0.0000

PRESSURE DROP PARAMETER:
HOT SIDE: 0.0000
COLD SIDE: 0.0000

BLOCK: MIX-100 MODEL: MIXER

-----------------------------------------
INLET STREAMS: S-115 S-114 S-113
OUTLET STREAM: S-119
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
IN OUT RELATIVE DIFF.
TOTAL BALANCE
MOLE(LBMOL/HR) 36372.3 36372.3 0.00000
MASS(LB/HR) 0.124500E+07 0.124500E+07 0.00000
ENTHALPY(BTU/HR) -0.583515E+10 -0.583515E+10 0.00000

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION 0.00000 LB/HR

*** INPUT DATA ***
TWO PHASE FLASH
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000
OUTLET PRESSURE: MINIMUM OF INLET STREAM PRESSURES
BLOCK: P-000  MODEL: PUMP

-------------------------------------
INLET STREAM:           S-000
OUTLET STREAM:          S-100
PROPERTY OPTION SET:   PENG-ROB  STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BALANCE</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>36372.6</td>
<td>36372.6</td>
</tr>
<tr>
<td>MASS(LB/HR )</td>
<td>0.124500E+07</td>
<td>0.124500E+07</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR )</td>
<td>-0.573013E+10</td>
<td>-0.573012E+10</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E             0.00000      LB/HR
PRODUCT STREAMS CO2E          0.00000      LB/HR
NET STREAMS CO2E PRODUCTION   0.00000      LB/HR
UTILITIES CO2E PRODUCTION     0.00000      LB/HR
TOTAL CO2E PRODUCTION         0.00000      LB/HR

*** INPUT DATA ***

PRESSURE CHANGE  PSI        2.00000
DRIVER EFFICIENCY          1.00000

FLASH SPECIFICATIONS:
LIQUID PHASE CALCULATION
NO FLASH PERFORMED
MAXIMUM NUMBER OF ITERATIONS     30
TOLERANCE                      0.000100000

*** RESULTS ***

VOLUMETRIC FLOW RATE  CUFT/HR       16,830.2
PRESSURE CHANGE  PSI              2.00000
NPSH AVAILABLE   FT-LBF/LB         27.2010
FLUID POWER  HP                    2.44803
BRAKE POWER  HP                    2.98844
ELECTRICITY  KW                    2.22848
PUMP EFFICIENCY USED              0.81917
NET WORK REQUIRED   HP             2.98844
HEAD DEVELOPED FT-LBF/LB          3.89325

BLOCK: R-100  MODEL: RYIELD
INLET STREAM: S-107
OUTLET STREAM: S-110
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

TOTAL BALANCE
MOLE(LBMOL/HR) 12124.2 12124.1 -0.102851 0.00000
MASS(LB/HR ) 415000. 415000. 0.00000
ENTHALPY(BTU/HR ) -0.187310E+10 -0.194673E+10 0.378200E-01

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION 0.00000 LB/HR

*** INPUT DATA ***
TWO PHASE TP FLASH
SPECIFIED TEMPERATURE F 212.000
SPECIFIED PRESSURE PSIA 14.6959
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

MASS-YIELD
SUBSTREAM MIXED :
WATER 0.474 GLUCOSE 0.526

*** RESULTS ***
OUTLET TEMPERATURE F 212.00
OUTLET PRESSURE PSIA 14.696
HEAT DUTY BTU/HR -0.73625E+08
VAPOR FRACTION 0.0000

V-L PHASE EQUILIBRIUM :

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WATER</td>
<td>0.90000</td>
<td>0.90000</td>
<td>1.0000</td>
<td>1.0028</td>
</tr>
</tbody>
</table>
GLUCOSE 0.99999E-01 0.99999E-01 0.23398E-06 0.21117E-05

**BLOCK: REF-500**  **MODEL: HEATER**

-----------------------------
INLET STREAM: S-521
OUTLET STREAM: S-508
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

<table>
<thead>
<tr>
<th></th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTAL BALANCE</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>705.706</td>
<td>705.706</td>
<td>0.00000</td>
</tr>
<tr>
<td>MASS(LB/HR)</td>
<td>74508.1</td>
<td>74508.1</td>
<td>0.00000</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.681302E+07</td>
<td>-0.897628E+07</td>
<td>0.240998</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

<table>
<thead>
<tr>
<th></th>
<th>FEED STREAMS CO2E</th>
<th>0.00000</th>
<th>LB/HR</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRODUCT STREAMS CO2E</td>
<td></td>
<td>0.00000</td>
<td>LB/HR</td>
</tr>
<tr>
<td>NET STREAMS CO2E PRODUCTION</td>
<td></td>
<td>0.00000</td>
<td>LB/HR</td>
</tr>
<tr>
<td>UTILITIES CO2E PRODUCTION</td>
<td></td>
<td>0.00000</td>
<td>LB/HR</td>
</tr>
<tr>
<td>TOTAL CO2E PRODUCTION</td>
<td>0.00000</td>
<td>0.00000</td>
<td>LB/HR</td>
</tr>
</tbody>
</table>

*** INPUT DATA ***

TWO PHASE TP FLASH

<table>
<thead>
<tr>
<th></th>
<th>SPECIFIED TEMPERATURE</th>
<th>F</th>
<th>-22.0000</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPECIFIED PRESSURE</td>
<td>PSIA</td>
<td>14.6959</td>
<td></td>
</tr>
<tr>
<td>MAXIMUM NO. ITERATIONS</td>
<td></td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>CONVERGENCE TOLERANCE</td>
<td></td>
<td>0.000100000</td>
<td></td>
</tr>
</tbody>
</table>

*** RESULTS ***

<table>
<thead>
<tr>
<th></th>
<th>OUTLET TEMPERATURE</th>
<th>F</th>
<th>-22.000</th>
</tr>
</thead>
<tbody>
<tr>
<td>OUTLET PRESSURE</td>
<td>PSIA</td>
<td>14.696</td>
<td></td>
</tr>
<tr>
<td>HEAT DUTY</td>
<td>BTU/HR</td>
<td>-0.21633E+07</td>
<td></td>
</tr>
<tr>
<td>OUTLET VAPOR FRACTION</td>
<td></td>
<td>0.0000</td>
<td></td>
</tr>
<tr>
<td>PRESSURE-DROP CORRELATION PARAMETER</td>
<td></td>
<td>0.0000</td>
<td></td>
</tr>
</tbody>
</table>

V-L PHASE EQUILIBRIUM :
CASTILLO, ERNST, LERCH, WINCHESTER

<table>
<thead>
<tr>
<th>COMP</th>
<th>F(I)</th>
<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-XYL</td>
<td>0.71989</td>
<td>0.71989</td>
<td>0.53386</td>
<td>0.26983E-03</td>
</tr>
<tr>
<td>O-XYL</td>
<td>0.33233E-01</td>
<td>0.33233E-01</td>
<td>0.18416E-01</td>
<td>0.20163E-03</td>
</tr>
<tr>
<td>M-XYL</td>
<td>0.69612E-01</td>
<td>0.69612E-01</td>
<td>0.47600E-01</td>
<td>0.24880E-03</td>
</tr>
<tr>
<td>N-HEX</td>
<td>0.32632E-09</td>
<td>0.32632E-09</td>
<td>0.13004E-07</td>
<td>0.14500E-01</td>
</tr>
<tr>
<td>ETHYLBEN</td>
<td>0.11709E-01</td>
<td>0.11709E-01</td>
<td>0.10614E-01</td>
<td>0.32981E-03</td>
</tr>
<tr>
<td>TOLUENE</td>
<td>0.10373</td>
<td>0.10373</td>
<td>0.36554</td>
<td>0.12822E-02</td>
</tr>
<tr>
<td>BENZENE</td>
<td>0.32811E-07</td>
<td>0.32811E-07</td>
<td>0.62054E-06</td>
<td>0.68814E-02</td>
</tr>
<tr>
<td>NAPTH</td>
<td>0.38125E-06</td>
<td>0.38125E-06</td>
<td>0.47681E-08</td>
<td>0.45507E-05</td>
</tr>
<tr>
<td>1:2:4-01</td>
<td>0.70387E-03</td>
<td>0.70387E-03</td>
<td>0.73988E-04</td>
<td>0.38248E-04</td>
</tr>
<tr>
<td>ISOPR-01</td>
<td>0.61117E-01</td>
<td>0.61117E-01</td>
<td>0.23867E-01</td>
<td>0.14209E-03</td>
</tr>
<tr>
<td>N-HEP-01</td>
<td>0.30016E-05</td>
<td>0.30016E-05</td>
<td>0.26459E-04</td>
<td>0.32074E-02</td>
</tr>
<tr>
<td>1-HEX-01</td>
<td>0.96289E-11</td>
<td>0.96289E-11</td>
<td>0.46729E-09</td>
<td>0.17658E-01</td>
</tr>
<tr>
<td>1-HEP-01</td>
<td>0.14550E-06</td>
<td>0.14550E-06</td>
<td>0.14170E-05</td>
<td>0.35434E-02</td>
</tr>
</tbody>
</table>

**BLOCK: SEP-300 MODEL: SEP**

Inlet Stream: S-323
Outlet Streams: S-325 S-313
Property Option Set: PENG-ROB STANDARD PR EQUATION OF STATE

### Mass and Energy Balance

<table>
<thead>
<tr>
<th>TOTAL BALANCE</th>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE (LBMOL/HR)</td>
<td>7810.82</td>
<td>7810.82</td>
<td>0.00000</td>
</tr>
<tr>
<td>MASS (LB/HR)</td>
<td>153817.</td>
<td>153817.</td>
<td>0.189210E-15</td>
</tr>
<tr>
<td>ENTHALPY (BTU/HR)</td>
<td>-0.526297E+09</td>
<td>-0.541065E+09</td>
<td>0.272937E-01</td>
</tr>
</tbody>
</table>

### CO2 Equivalent Summary

| FEED STREAMS CO2E | 93678.2 | LB/HR |
| PRODUCT STREAMS CO2E | 93678.2 | LB/HR |
| NET STREAMS CO2E PRODUCTION | 0.00000 | LB/HR |
| UTILITIES CO2E PRODUCTION | 0.00000 | LB/HR |
| TOTAL CO2E PRODUCTION | 0.00000 | LB/HR |

*** Input Data ***

Flash Specs for Stream S-325
Two Phase TP Flash
Pressure Drop PSI 0.0
Maximum No. Iterations 30
CONVERGENCE TOLERANCE 0.000100000

FLASH SPECS FOR STREAM S-313
TWO PHASE TP FLASH
PRESSURE DROP PSI 0.0
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

FRACTION OF FEED
SUBSTREAM= MIXED
STREAM= S-313 CPT= PROPANE FRACTION= 1.00000
CO2 1.00000
H2 0.0

*** RESULTS ***

HEAT DUTY BTU/HR -0.14768E+08

COMPONENT = PROPANE
STREAM SUBSTREAM SPLIT FRACTION
S-313 MIXED 1.00000

COMPONENT = CO2
STREAM SUBSTREAM SPLIT FRACTION
S-313 MIXED 1.00000

COMPONENT = WATER
STREAM SUBSTREAM SPLIT FRACTION
S-313 MIXED 1.00000

COMPONENT = H2
STREAM SUBSTREAM SPLIT FRACTION
S-325 MIXED 1.00000

BLOCK: SPT-100 MODEL: FSPLIT
-----------------------------------
INLET STREAM: S-100
OUTLET STREAMS: S-101 S-102 S-103
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***
CASTILLO, ERNST, LERCH, WINCHESTER

TOTAL BALANCE

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>36372.6</td>
<td>36372.6</td>
</tr>
<tr>
<td>MASS(LB/HR)</td>
<td>0.124500E+07</td>
<td>0.124500E+07</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.573012E+10</td>
<td>-0.573012E+10</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION 0.00000 LB/HR

*** INPUT DATA ***

FRACTION OF FLOW STRM=S-101 FRAC= 0.33333
STRM=S-102 FRAC= 0.33333

*** RESULTS ***

STREAM= S-101 SPLIT= 0.33333 KEY= 0 STREAM-ORDER= 1
S-102 0.33333 0 2
S-103 0.33333 0 3

BLOCK: VAL-200 MODEL: VALVE

--------------
INLET STREAM: S-224
OUTLET STREAM: S-225
PROPERTY OPTION SET: PENG-ROB STANDARD PR EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

TOTAL BALANCE

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLE(LBMOL/HR)</td>
<td>36374.4</td>
<td>36374.4</td>
</tr>
<tr>
<td>MASS(LB/HR)</td>
<td>0.125242E+07</td>
<td>0.125242E+07</td>
</tr>
<tr>
<td>ENTHALPY(BTU/HR)</td>
<td>-0.597601E+10</td>
<td>-0.597601E+10</td>
</tr>
</tbody>
</table>

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 LB/HR
PRODUCT STREAMS CO2E 0.00000 LB/HR
NET STREAMS CO2E PRODUCTION 0.00000 LB/HR
UTILITIES CO2E PRODUCTION 0.00000 LB/HR
TOTAL CO2E PRODUCTION  0.00000  LB/HR

*** INPUT DATA ***

VALVE OUTLET PRESSURE  PSIA  741.696
VALVE FLOW COEF CALC.  NO

FLASH SPECIFICATIONS:
NPHASE  2
MAX NUMBER OF ITERATIONS  30
CONVERGENCE TOLERANCE  0.000100000

*** RESULTS ***

VALVE PRESSURE DROP  PSI  418.606